Skoltech
Skolkovo Institute of Science and Technology

Energy Colloquium

September 27, 2016

Perspectives of exascale computing for novel energy technologies

Vladimir Stegailov

Joint Institute for High Temperatures of RAS

ИВТАН

MIPT
MOSCOW INSTITUTE OF PHYSICS AND TECHNOLOGY

ВЫСШАЯ ШКОЛА ЭКОНОМИКИ

Развитие вычислительной техники

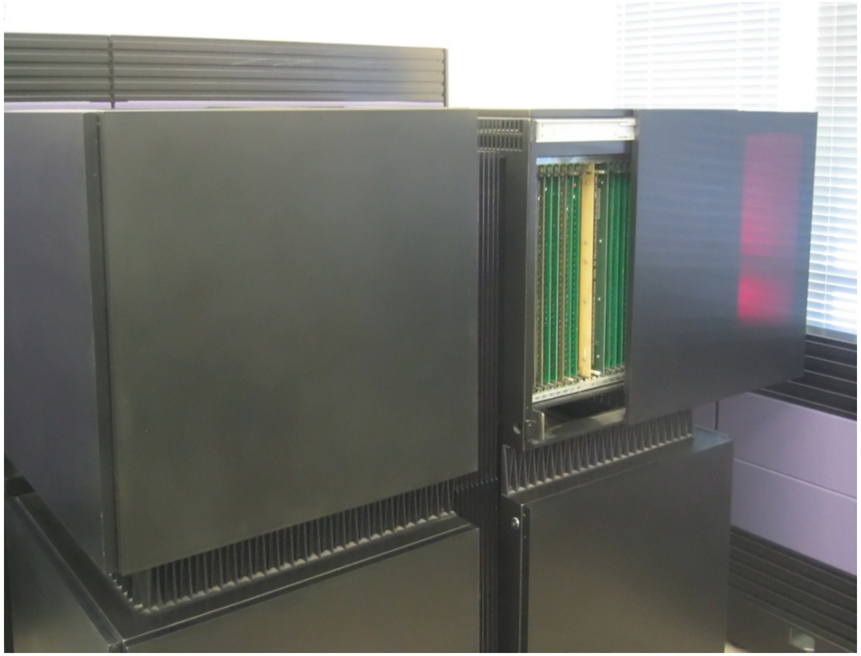
CDC 3600

peak: 367000 GFlops
131072 CPUs
- clock fq.: 700 MHz
- memory: 250 Mb

Blue Gene/L

peak: 0.0013 GFlops
1 CPU
- clock fq.: 0.7 MHz
- memory: 32 Kb

Суперкомпьютеры 1986-87 гг.



Thinking Machines CM-2:
16384 однобитовых процессора совместно с 512 арифметическими ускорителями Weitek

Meiko Computing Surface:
64 транспьютерных узлов с процессорами Intel i860

В. В. Стегайлов, Г. Э. Норман. Проблемы развития суперкомпьютерной отрасли в России: взгляд пользователя высокопроизводительных систем // Программные системы: теория и приложения: электрон. научн. журн. 2014. Т. 5, № 1(19), с. 111–152. URL: http://psta.psiras.ru/read/psta2014_1_111-152.pdf

… и параллельные алгоритмы для первопринципных расчетов

VOLUME 68, NUMBER 9 PHYSICAL REVIEW LETTERS 2 MARCH 1992

Ab Initio Theory of the Si(111)-(7×7) Surface Reconstruction: A Challenge for Massively Parallel Computation

Karl D. Brommer,[1] M. Needels,[2] B. E. Larson,[3] and J. D. Joannopoulos[1]

[1]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
[2]*AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, New Jersey 07974*
[3]*Thinking Machines, Cambridge, Massachusetts 02139*
(Received 8 November 1991)

An *ab initio* investigation of the Si(111)-(7×7) surface reconstruction is undertaken using the state of the art in massively parallel computation. Calculations of the total energy of an ∼700 effective-atom supercell are performed to determine (1) the fully relaxed atomic geometry, (2) the scanning tunneling microscope images as a function of bias voltage, and (3) the energy difference between the (7×7) and the (2×1) reconstructions. The (7×7) reconstruction is found to be energetically favorable to the (2×1) surface by 60 meV per (1×1) unit cell.

PACS numbers: 73.20.−r, 68.35.Bs, 68.35.Md

Thinking Machines CM-2

VOLUME 68, NUMBER 9 PHYSICAL REVIEW LETTERS 2 MARCH 1992

Ab Initio Total-Energy Calculations for Extremely Large Systems: Application to the Takayanagi Reconstruction of Si(111)

I. Štich, M. C. Payne, R. D. King-Smith, and J-S. Lin
Cavendish Laboratory (TCM), University of Cambridge, Madingley Road, Cambridge CB3 0HE, United Kingdom

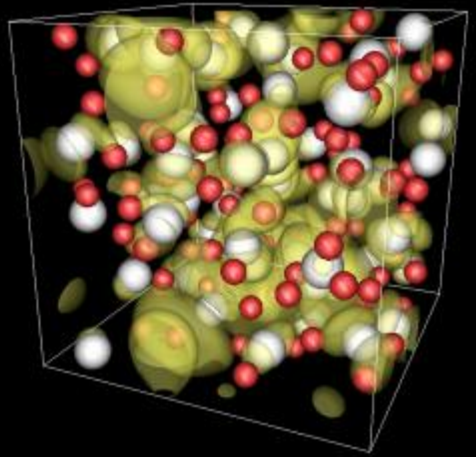
L. J. Clarke
Edinburgh Parallel Computer Centre, University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, United Kingdom
(Received 8 November 1991)

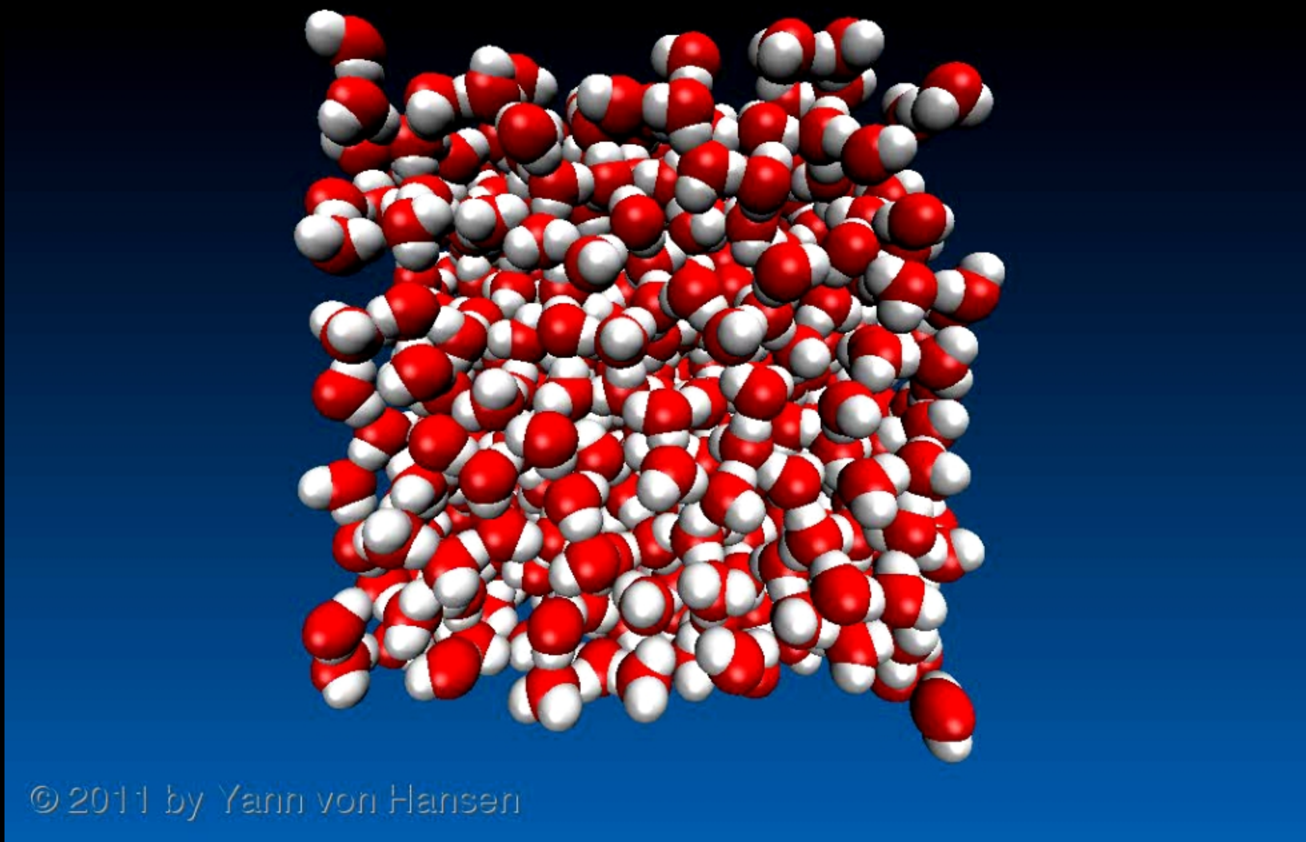
We have implemented a set of total-energy pseudopotential codes on a parallel computer which allows calculations to be performed for systems containing many hundreds of atoms in the unit cell. Using these codes we have calculated the total energies and structures of the 3×3, 5×5, and 7×7 Takayanagi reconstructions of the (111) surface of silicon. We find that the 7×7 structure minimizes the surface energy and observe structural trends across the series which can be correlated with the degree of charge transfer between the dangling bonds on the adatoms and rest atoms.

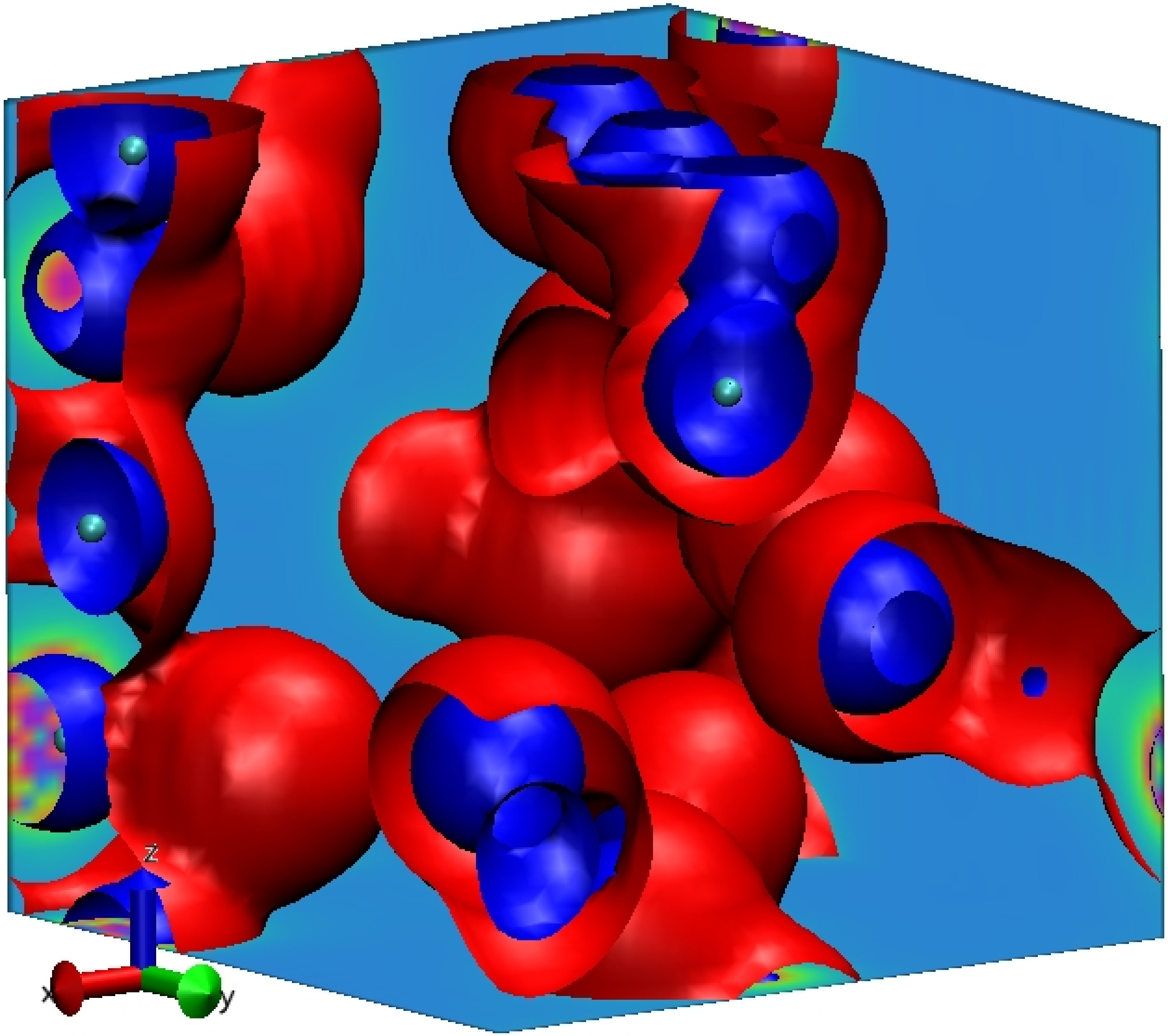
PACS numbers: 68.35.−p, 31.20.−d, 71.45.Nt

Meiko Computing Surface

Атомистические модели воды

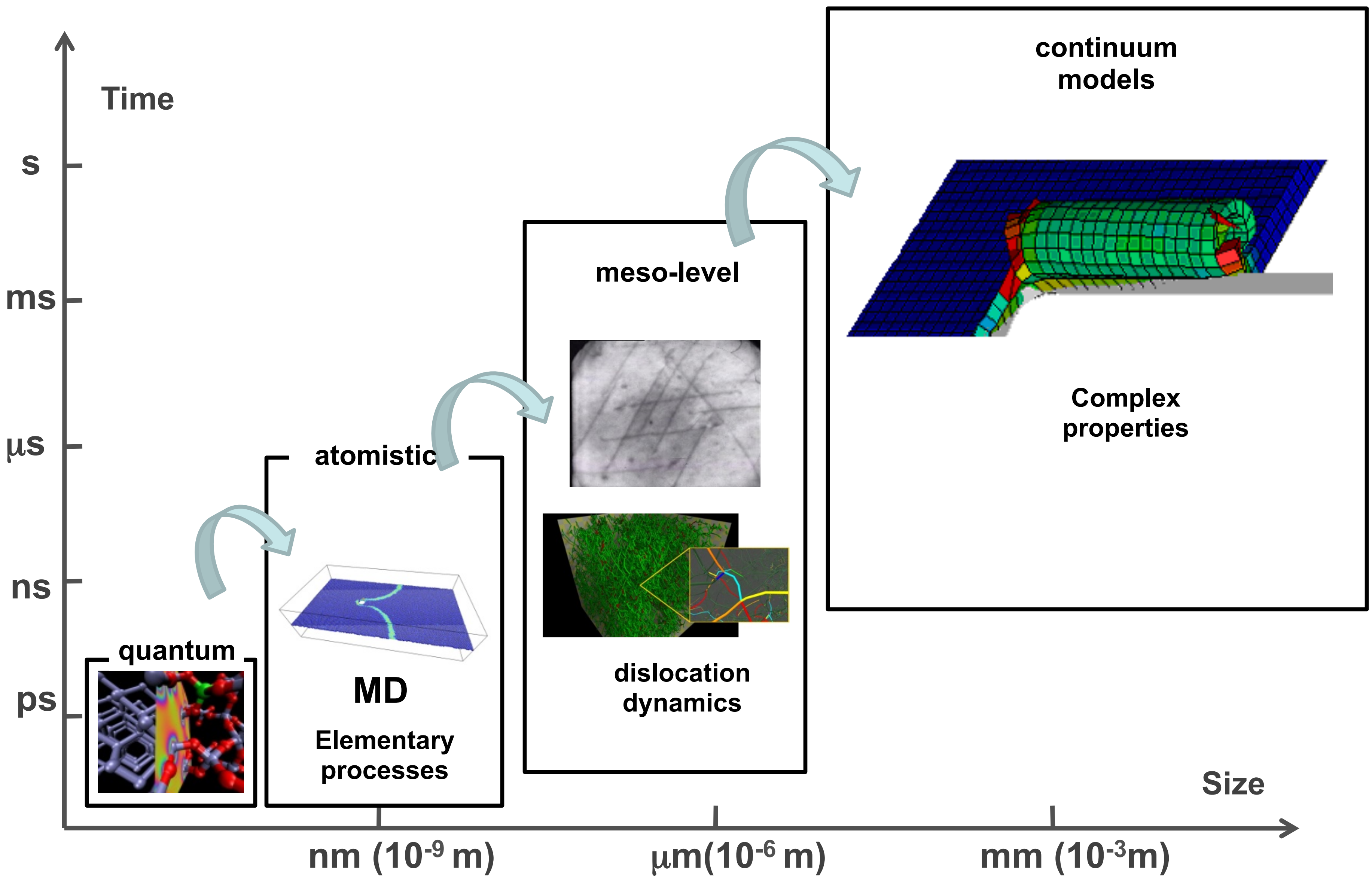






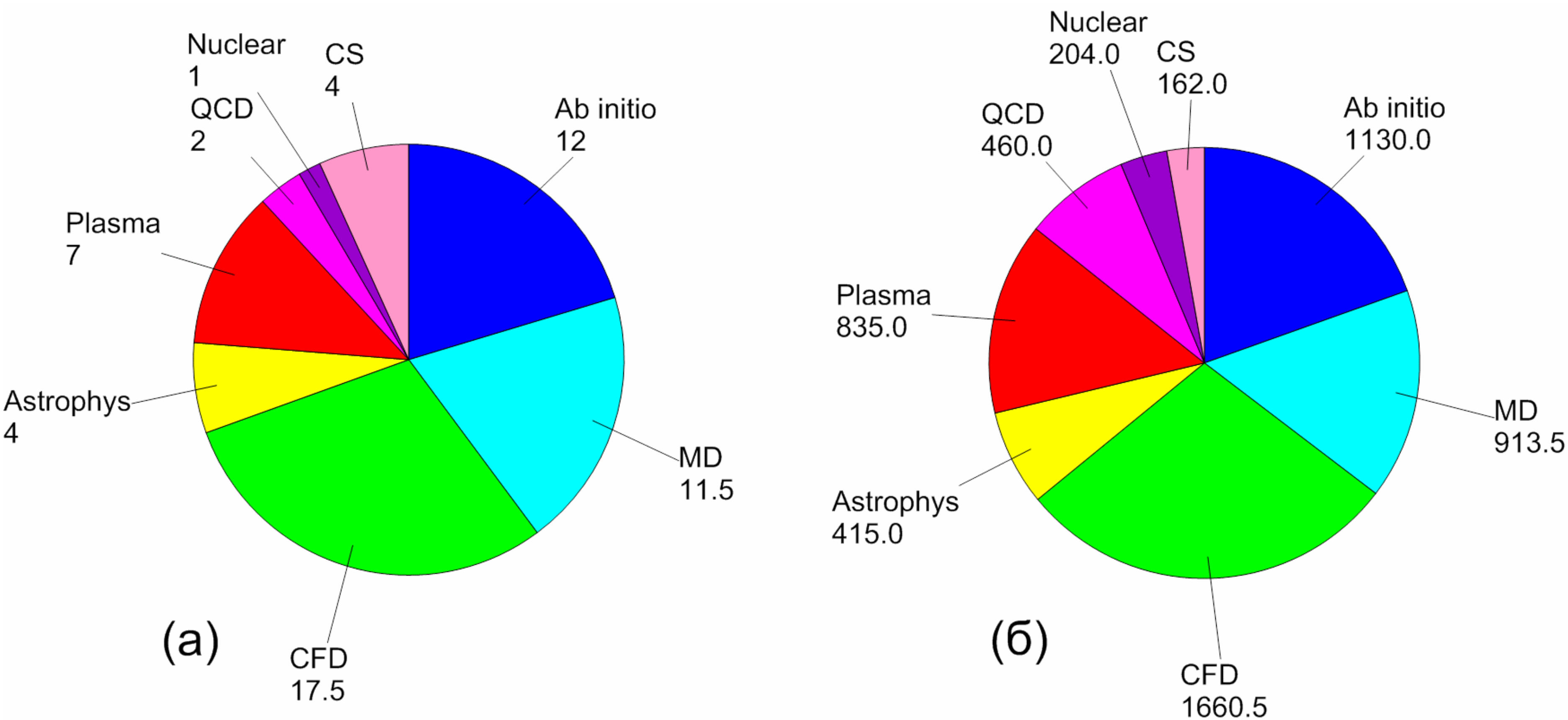
Norman, G., Saitov, I., Stegailov, V., & Zhilyaev, P. (2015). Ab initio calculation of shocked xenon reflectivity. Physical Review E, 91(2), 023105.

Многомасштабный подход в теории и моделировании



Деление проектов INCITE 2014 г. по тематикам

Innovative and Novel Computational Impact on Theory and Experiment



Число проектов по каждой тематике

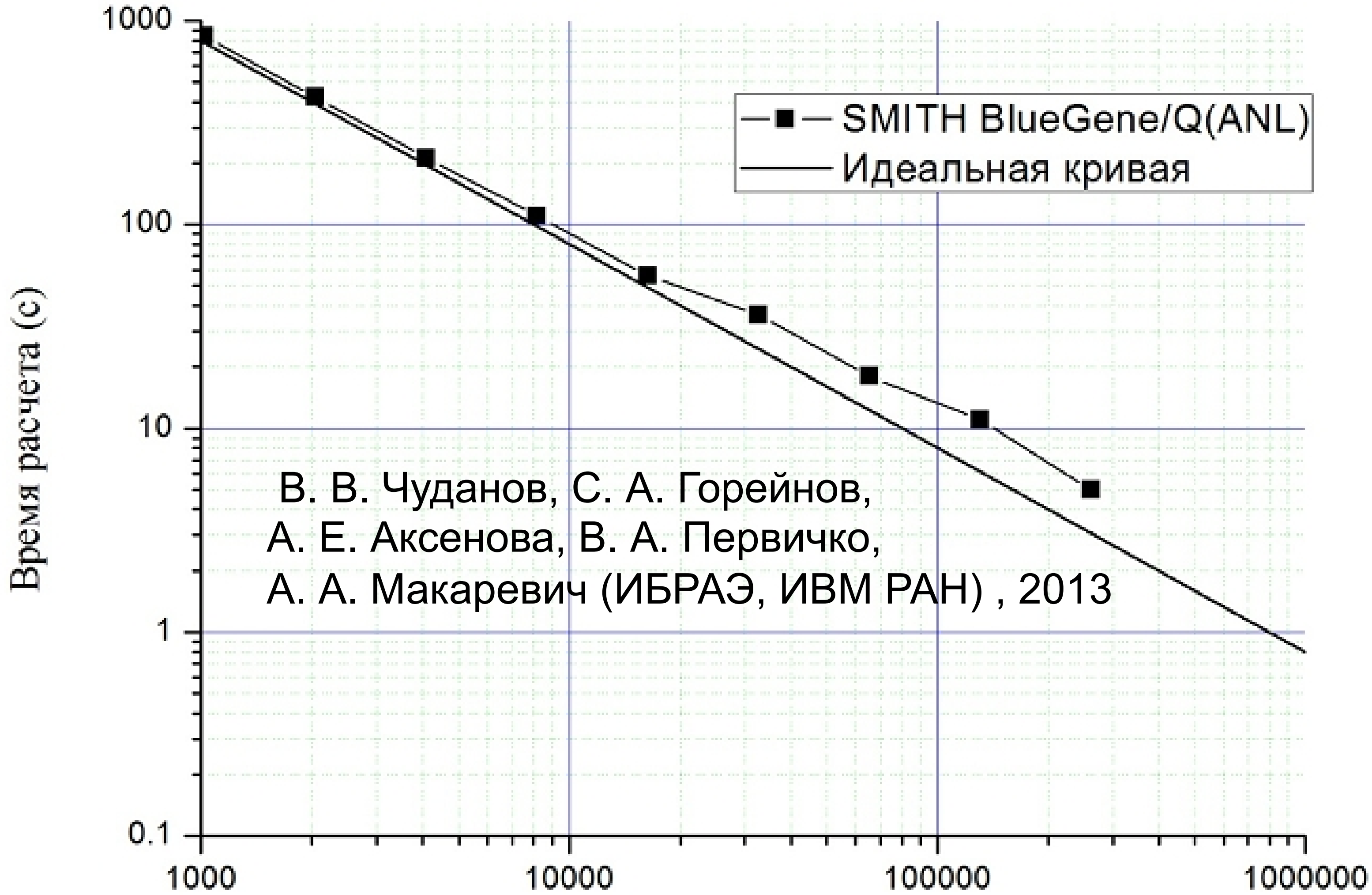
Выделенное на каждую тематику вычислительное время в миллионах процессоро-часов

Г. Э. Норман, Н. Д.Орехов, В. В. Писарев, Г. С. Смирнов и др. «Зачем и какие суперкомпьютеры экзафлопсного класса нужны в естественных науках», Программные системы: теория и приложения, 2015, 6:4(27), с. 243–311. URL: http://psta.psiras.ru/read/psta2015_4_243-311.pdf

Computational fluid dynamics

SMITH: «сильная» масштабируемость, $\frac{p_0 T(N,p_0)}{pT(N,p)}$.

Ниже $p_0 = 1024$, максимальное $p = 262144$, $N = 4097^3$. Сплошная линия соответствует зависимости $T = p_0 T(N, p_0)/p$.



В. В. Чуданов, С. А. Горейнов, А. Е. Аксенова, В. А. Первичко, А. А. Макаревич (ИБРАЭ, ИВМ РАН) , 2013

Estimates from the ISC-2015 Conference

Rough estimate of DNS flow over an aircraft

An airbus 310 cruising at 250 m/s at 10000 m

For 1 second of simulated flight:
1 teraflops machine – $8*10^5$ years
50 exaflops machine – 1 weak

(based on John Kim, TSFP-9, 2015)

EU PRACE initiative

US DOE INCITE initiative

Innovative & Novel Computational Impact on Theory and Experiment

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

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Leading the way for Scientific Computing

INCITE supports computationally intensive, large-scale research projects with large amounts of dedicated time on supercomputers at DOE's Leadership Computing Facilities. Learn More

	DOE	University	Government	Industry	International
DOE	**12**	14	1	0	1
University		**17**	0	3	2
Government			**0**	0	1
Industry				**1**	0
International					**3**

University-DOE-Industry	2
University-DOE-International	3

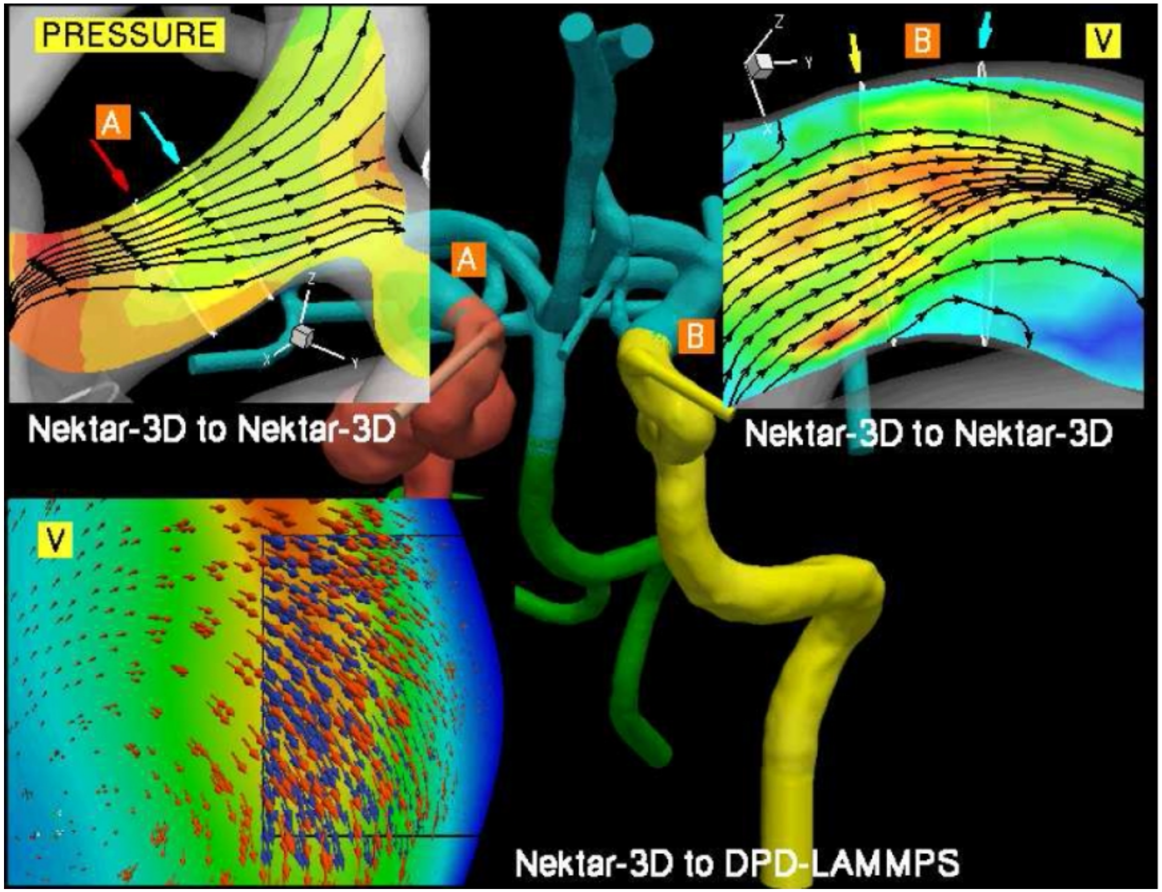
US DOE INCITE initiative

Год	Всего проектов	Проекты по молекулярному и атомистическому моделированию	% от общего числа
2006	15	6	40%
2007	45	11	24%
2008	58	16	28%
2009	66	20	30%
2010	70	23	33%
2011	57	18	32%
2012	60	23	38%
2013	61	24	39%

2012 год:
60 проектов = 1672 миллиона процессор-часов на IBM BlueGene/P и Cray XT5
23 проекта по молекулярному и атомистическому моделированию = 518 млн. час.
31 % общего времени

US DOE INCITE initiative

Пример результатов комбинированного расчета кровотока с эффектами отложения холестериновых бляшек в рамках многомасштабной модели, сочетающей атомистическое моделирование с моделью жидкости Навье-Стокса



Grinberg L., et al. **A new computational paradigm in multiscale simulations: Application to brain blood flow** // Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC), 2011.

US DOE INCITE initiative

Демонстрация сохранения эффективности распараллеливания решения одной задачи на системах BlueGene/P и Cray XT5

Число ядер	Время загрузки ЦПУ, с	Эффективность
BlueGene/P (4 ядра на узел)		
28 672	3205.58	
61 440	1399.12	1.07
126 976	665.79	1.02
Cray XT5 (12 ядер на узел)		
17 280 (Kraken)	2194	
25 920 (Kraken)	1177	1.24
34 560 (Jaguar)	806	1.10
93 312 (Jaguar)	280	1.07
186 624 (Jaguar)	206	0.68

Grinberg L., et al. **A new computational paradigm in multiscale simulations: Application to brain blood flow** // Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC), 2011.

Пример из INCITE 2014

Type:	New
Title:	"Computational Actinide Chemistry: Reliable Predictions and New Concepts"

Principal Investigator:	David Dixon, The University of Alabama & Argonne National Laboratory
Co-Investigators:	Jochen Autschbach, University at Buffalo, State University of New York Enrique Batista, Los Alamos National Laboratory Aurora Clark, Washington State University Wibe de Jong, Lawrence Berkeley National Laboratory Laura Gagliardi, The University of Minnesota Jeff Hammond, Argonne National Laboratory Richard Martin, Los Alamos National Laboratory Kirk Peterson, Washington State University Gustavo Scuseria, Rice University
Scientific Discipline:	Chemistry: Physical
INCITE Allocation:	**250,000,000 processor hours**
Site:	Oak Ridge National Laboratory
Machine (Allocation):	Cray XK7 (150,000,000 processor hours)
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (100,000,000 processor hours)

Пример из INCITE 2014

Type: New
Title: "Cosmological Simulations for Large-Scale Sky Surveys"

Principal Investigator: Salman Habib, Argonne National Laboratory

Scientific Discipline: Physics: High Energy Physics

INCITE Allocation: **200,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (100,000,000 processor hours)

Пример из INCITE 2014

Type:	Renewal
Title:	"High-fidelity Simulation of Tokamak Edge Plasma Transport"

Principal Investigator:	Choong-Seock Chang, Princeton Plasma Physics Laboratory
Co-Investigators:	Stephane Ethier, Princeton Plasma Physics Laboratory
	Scott Klasky, Oak Ridge National Laboratory
	Robert Moser, The University of Texas at Austin
	Scott Parker, University of Colorado
	Mark Shephard, Rensselaer-Polytechnic Institute
	Pat Worley, Oak Ridge National Laboratory
Scientific Discipline:	Physics: Plasma Physics
INCITE Allocation:	**229,000,000 processor hours**
Site:	Oak Ridge National Laboratory
Machine (Allocation):	Cray XK7 (129,000,000 processor hours)
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (100,000,000 processor hours)

Пример из INCITE 2014

Type:	New
Title:	"Lattice QCD"
Principal Investigator:	Paul Mackenzie, Fermi National Accelerator Laboratory
Co-Investigators:	Richard Brower, Boston University Norman Christ, Columbia University Frithjof Karsch, Brookhaven National Laboratory Julius Kuti, University of California, San Diego John Negele, Massachusetts Institute of Technology David Richards, Jefferson National Laboratory Martin Savage, University of Washington Robert Sugar, University of California, Santa Barbara
Scientific Discipline:	Physics: Particle Physics
INCITE Allocation:	**340,000,000 processor hours**
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (240,000,000 processor hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	Cray XT (100,000,000 processor hours)

Пример из INCITE 2014

Type: New
Title: "Nuclear Structure and Nuclear Reactions"

Principal Investigator:	James Vary, Iowa State University
Co-Investigators:	Joseph Carlson, Los Alamos National Laboratory
	Gaute Hagen, Oak Ridge National Laboratory
	Pieter Maris, Iowa State University
	Hai Ah Nam, Oak Ridge National Laboratory
	Petr Navratil, TRIUMF
	Witold Nazarewicz, University of Tennessee-Knoxville
	Steven Pieper, Argonne National Laboratory
	Nicolas Schunck, Lawrence Livermore National Laboratory
Scientific Discipline:	Physics: Nuclear Physics
INCITE Allocation:	**204,000,000 processor hours**
Site:	Oak Ridge National Laboratory **Machine**
(Allocation):	Cray XK7 (104,000,000 processor hours)
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (100,000,000 processor hours)

Пример из INCITE 2014

Type:	New
Title:	"Petascale Simulations of Self-Healing Nanomaterials"

Principal Investigator:	Rajiv Kalia, University of Southern California
Co-Investigator:	Aiichiro Nakano, University of Southern California
Scientific Discipline:	Materials Science: Condensed Matter and Materials
INCITE Allocation:	**200,000,000 processor hours**
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (200,000,000 processor hours)

Пример из INCITE 2014

Type:	New
Title:	"QMC Simulations Database for Predictive Modeling and Theory"

Principal Investigator:	Jeongnim Kim, Oak Ridge National Laboratory
Co-Investigators:	David Ceperley, University of Illinois at Urbana-Champaign
	Jeffrey Greeley, Purdue University
	Burkhard Militzer, University of California, Berkeley
	Miguel Morales, Lawrence Livermore National Laboratory
	Luke Shulenburger, Sandia National Laboratories
Scientific Discipline:	Materials Science: Condensed Matter and Materials
INCITE Allocation:	**200,000,000 processor hours**
Site:	Oak Ridge National Laboratory **Machine**
(Allocation):	Cray XK7 (100,000,000 processor hours)
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (100,000,000 processor hours)

Пример из INCITE 2014

Type:	Renewal
Title:	"Simulation of Laser-Plasma Interaction in National Ignition Facility Experiments"

Principal Investigator:	Steven Langer, Lawrence Livermore National Laboratory
Co-Investigators:	Denise Hinkel, Lawrence Livermore National Laboratory
Scientific Discipline:	Physics: Plasma Physics
INCITE Allocation:	**200,000,000 processor hours**
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (200,000,000 processor hours)

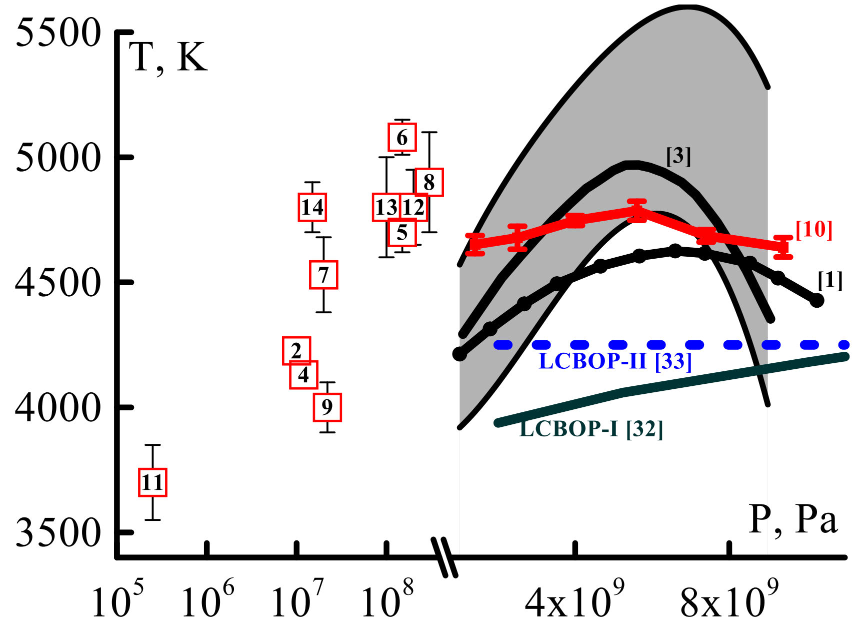
Пример из INCITE 2014

Type:	New
Title:	"Solving Petascale Public Health and Safety Problems Using Uintah"
Principal Investigator:	Martin Berzins, University of Utah
Co-Investigator:	Todd Harman, University of Utah
	John Schmidt, University of Utah
	Jennifer Spinti, University of Utah
	Jeremy Thornock, University of Utah
	Charles Wight, Weber State University
Scientific Discipline:	Chemistry: Combustion
INCITE Allocation:	**200,000,000 processor hours**
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/Q (200,000,000 processor hours)

Плавление графита

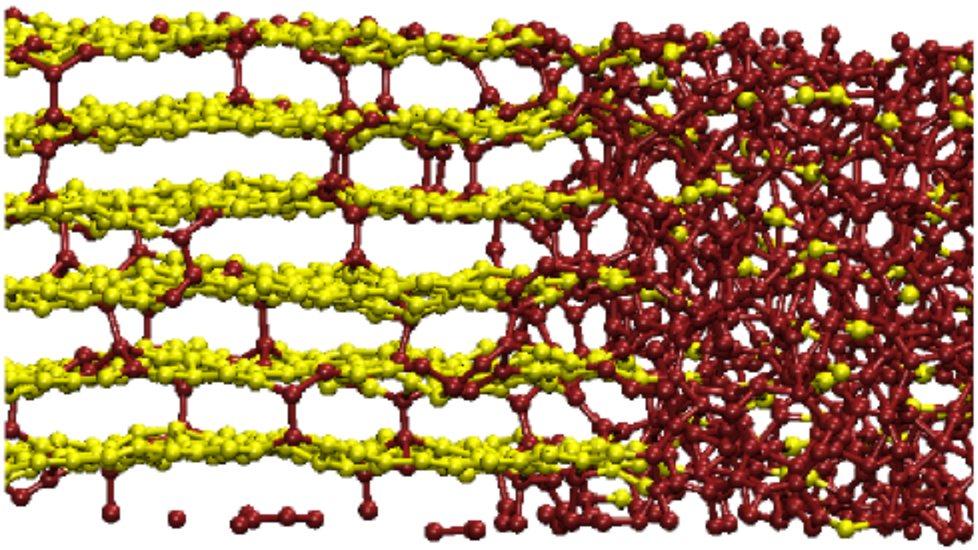
Orekhov N.D., Stegailov V.V. Graphite melting: Atomistic kinetics bridges theory and experiment // Carbon. 2015. V. 87. P. 358-364.

Кривая плавления графита: экспериментальные результаты

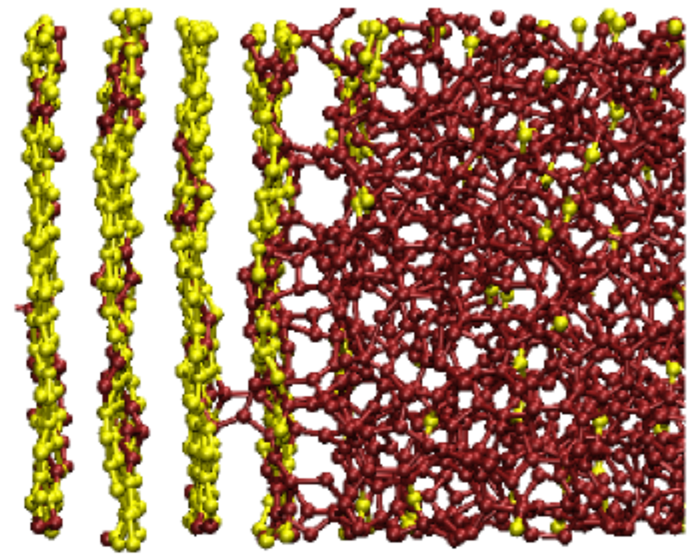


[1] *F. P. Bundy,* **J. Chem. Phys.** 38, 618 **(1963)**.
[2] *G. J. Schoessow,* **Phys. Rev. Lett.** 21, 738 **(1968)**.
[3] *N. S. Fateeva and L. F. Vereshchagin,* **JETP Lett.** 13, 110 **(1971)**.
[4] *N. A. Gokcen, E. T. Chang, T. M. Poston, and D. J. Spencer,* **High. Temp. Sci.** 8, 81 **(1976)**.
[5] *M. A. Sheindlin and V. N. Senchenko,* **Sov. Phys. Dokl.** 298, 1383 **(1988)**.
[6] *A. V. Baitin, A. A. Lebedev, S. V. Romanenko, V. N. Senchenko, and M. A. Sheindlin,* **High Temp. High Pres.** 22, 157 **(1990)**.
[7] *A. Cezairliyan and A. P. Miiller,* **Int. J. Thermophys.** 11, 643 **(1990)**.
[8] *G. Pottlacher, R. S. Hixson, S. Melnitzky, E. Kaschnitz, M. A. Winkler, and H. Jager,* **Thermochim. Acta** 218, 183 **(1993)**.
[9] *E. I. Asinovskij, A. V. Kirillin, and A. V. Kostanovskij,* **High. Temp.** 35, 716 **(1997)**.
[10] *M. Togaya*, **Phys. Rev. Lett.** 79, 2474 **(1997)**.
[11] *E. I. Asinovskii, A. V. Kirillin, A. V. Kostanovskii, and V. E. Fortov*, **High. Temp.** 36, 716 **(1998)**.
[12] *M. Musella, C. Ronchi, M. V. Brykin, and M. A. Sheindlin*, **J. Appl. Phys.** 84, 2530 **(1998)**.
[13] *A. I. Savvatimskii*, **Physics-Uspekhi** 46, 1295 **(2003)**.
[14] *A. Y. Basharin, M. V. Brykin, M. Y. Marin, I. S. Pakhomov, and S. F. Sitnikov*, **High. Temp**. 42, 60 **(2004)**.
[32] *L. M. Ghiringhelli, J. H. Los, E. J. Meijer, A. Fasolino, and D. Frenkel,* **Phys. Rev. Lett.** 94, 145701 **(2005)**.
[33] *F. Colonna, J. H. Los, A. Fasolino, and E. J. Meijer,* **Phys. Rev. B** 80, 1 **(2009)**.

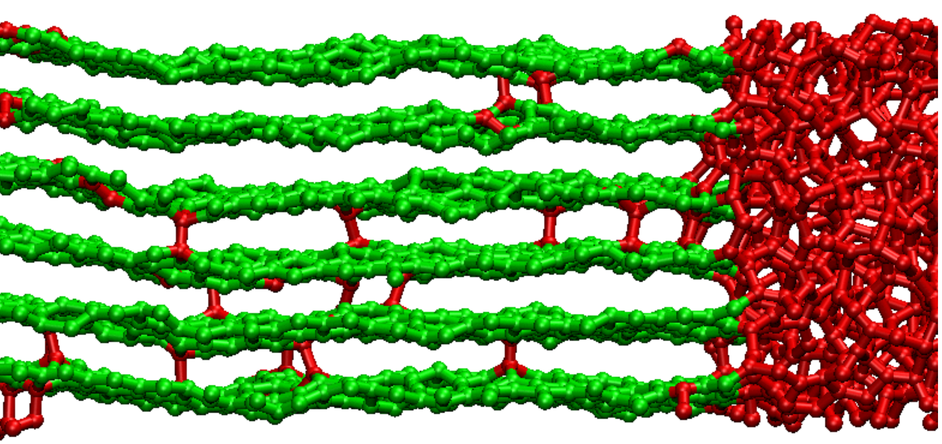
Melting front propagation in two-phase model

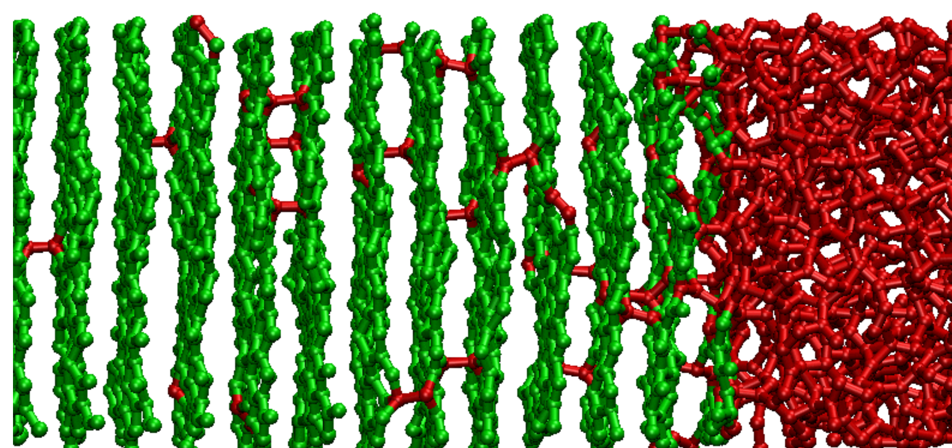


A

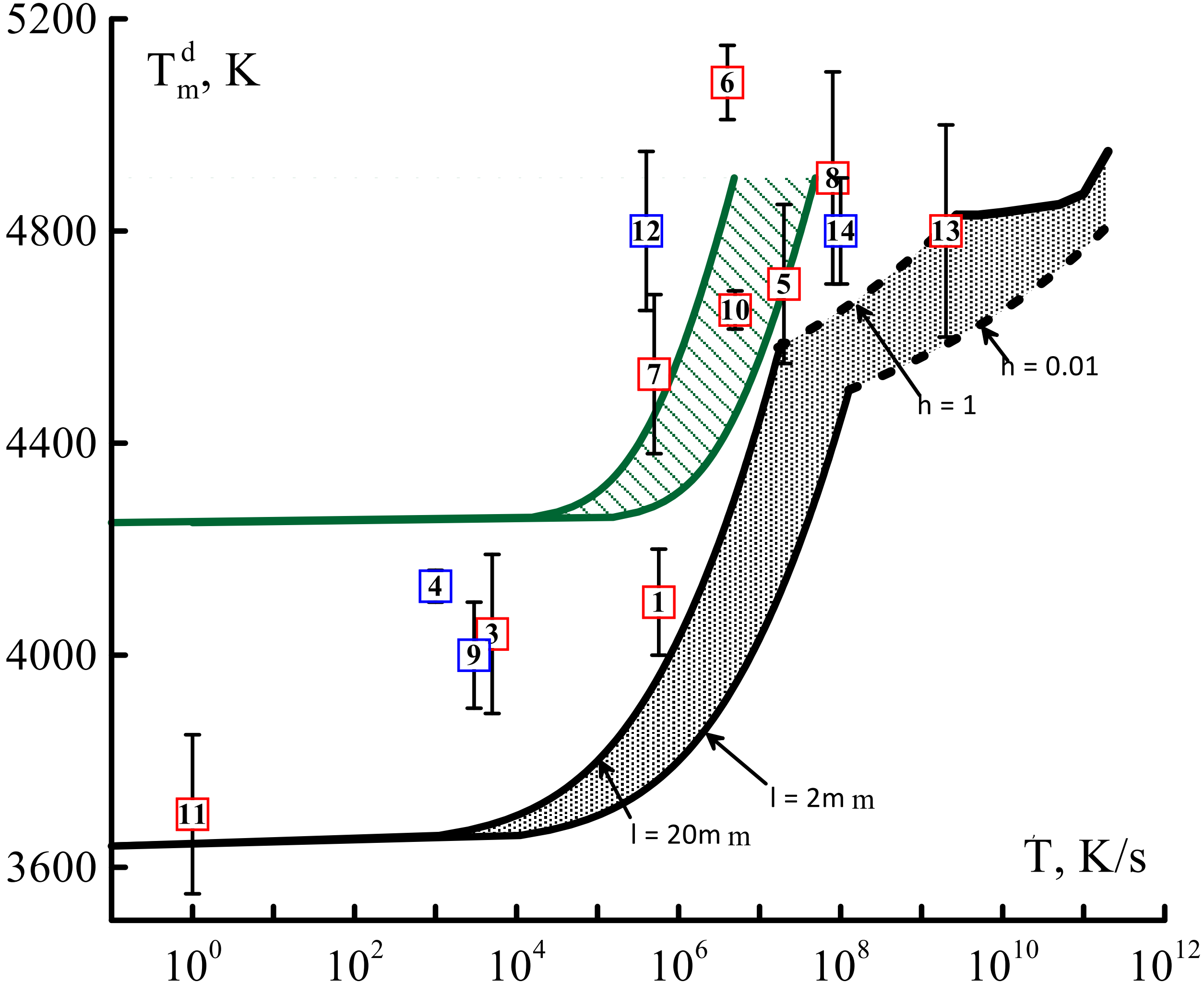


B





Фиксируемая в эксперименте “температура плавления” графита в зависимости от скорости нагрева



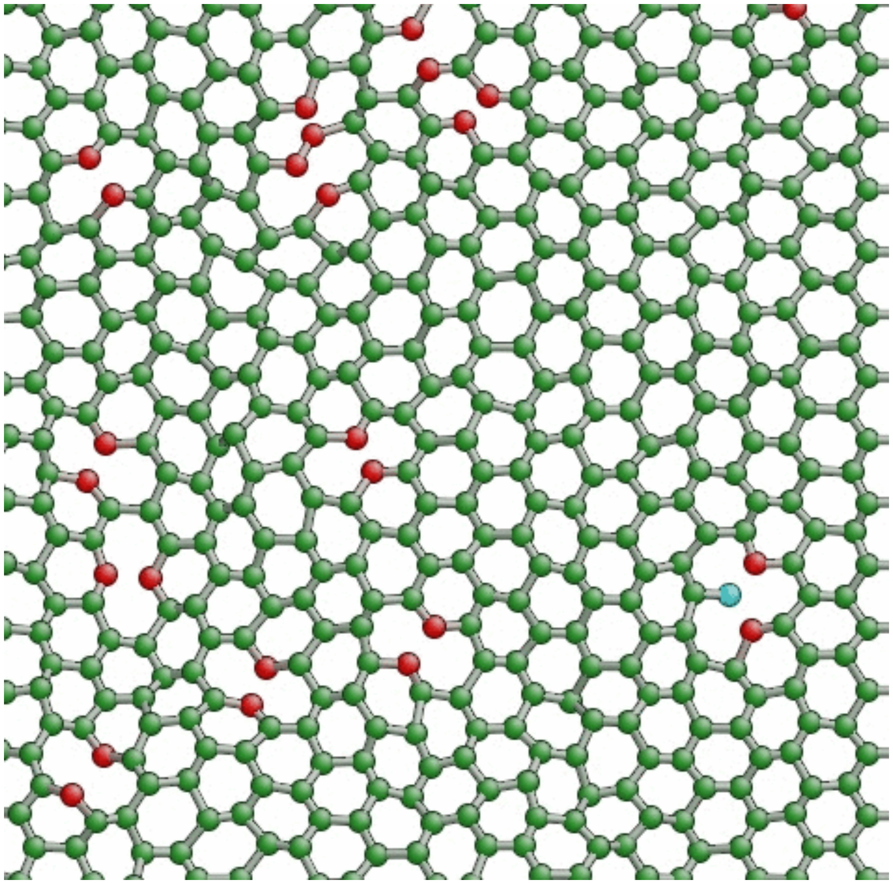
Нагрев током

Лазерный нагрев

AIREBO
(Tm = 3640 ± 150 K)

LCBOP-II
(Tm = 4250 ± 50 K)

Melting of a single graphene plane



- 1-fold
- 2-fold
- 3-fold

T = 4950 K

Cluster of Stone–Wales defects

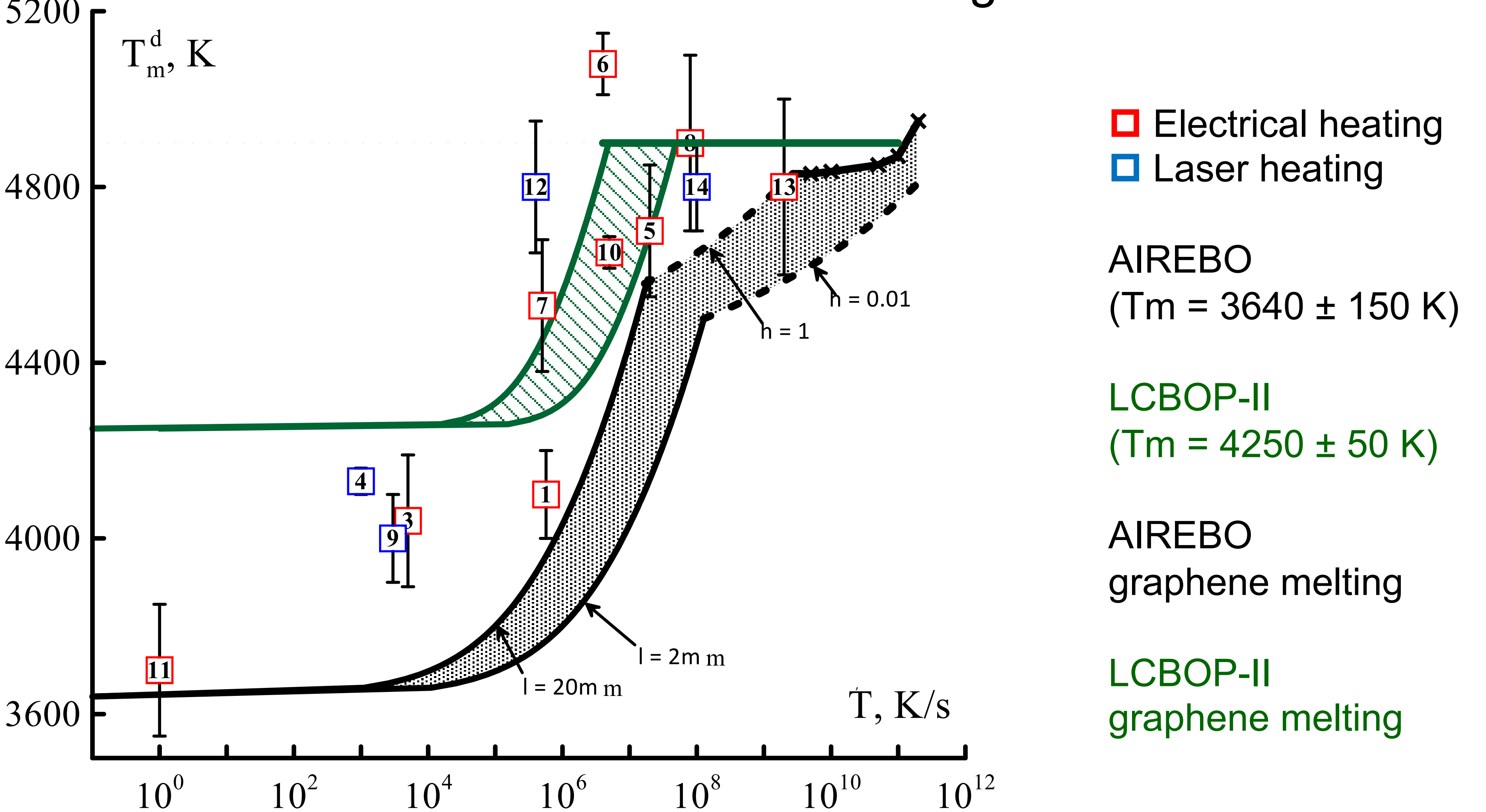
AIREBO: Tmelt = 4850 - 4900 K

LCBOP II [1]: Tmelt ≈ 4900 K [2]

[1] L Ghiringhelli, J Los, E Meijer, A Fasolino, D Frenkel // PRL **94** (2005) 145701

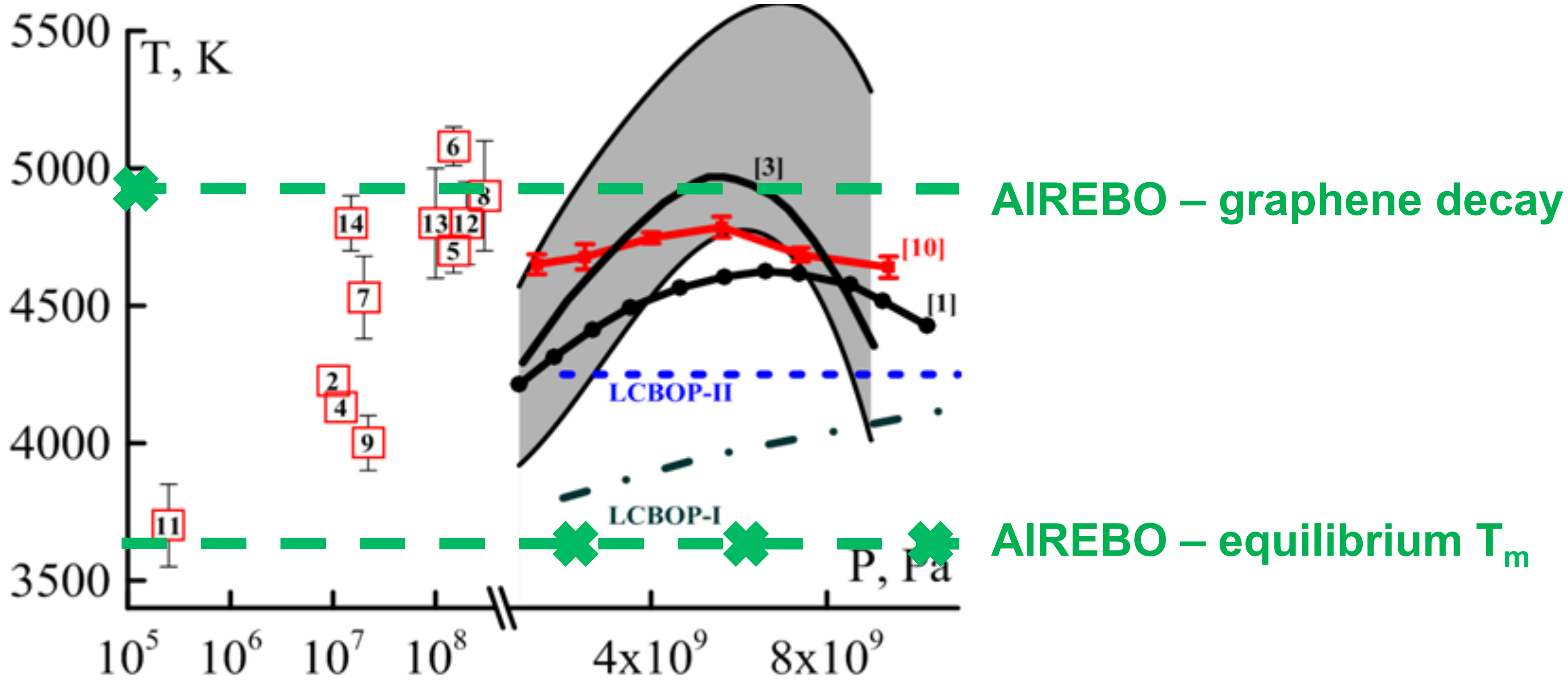
[2] K V Zakharchenko, A Fasolino, J H Los and M I Katsnelson // J. Phys.: Condens. Matter **23** (2011) 202202

Experimentally detected "melting temperature" of graphite as a function of heating rate



These results suggest that at the heating rates higher that ~10^6 K/s graphite specimens in most cases become superheated, the solid-liquid transition temperature becomes higher than the equilibrium melting temperature and is influenced mainly by the specimen microstructure and the energy deposition process.

Pressure dependence of the melting temperature



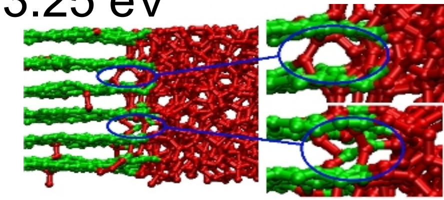
1. Experimental data for $T_m(P)$ were obtained for porous samples (1.6 g/cc)
2. Porous samples under pressure →

   → change in the average interplanar distance →

   → change in W_f →

   → change in the "experimentally observed" temperature of melting
3. Thus melting curve maximum can be explained as a kinetic and structural effect

W_f ~ 3.25 eV



Свойства материалов ядерной энергетики (ядерные топлива)

Накопление повреждение в топливах: образование пузырей

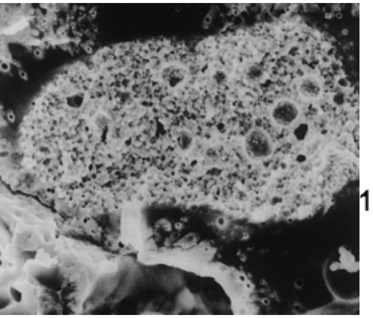
Точки – эксперимент для UO_2

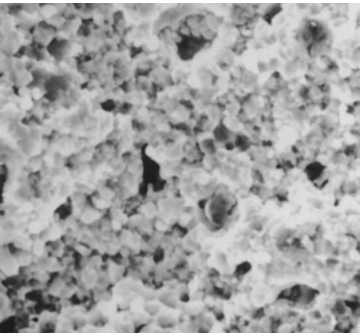
Линии – кинетическая модель

$$\frac{dc_i}{dt} = G - k_v^2 D_i c_i - k_i^2 D_v c_v - k_{is}^2 D_i c_i,$$

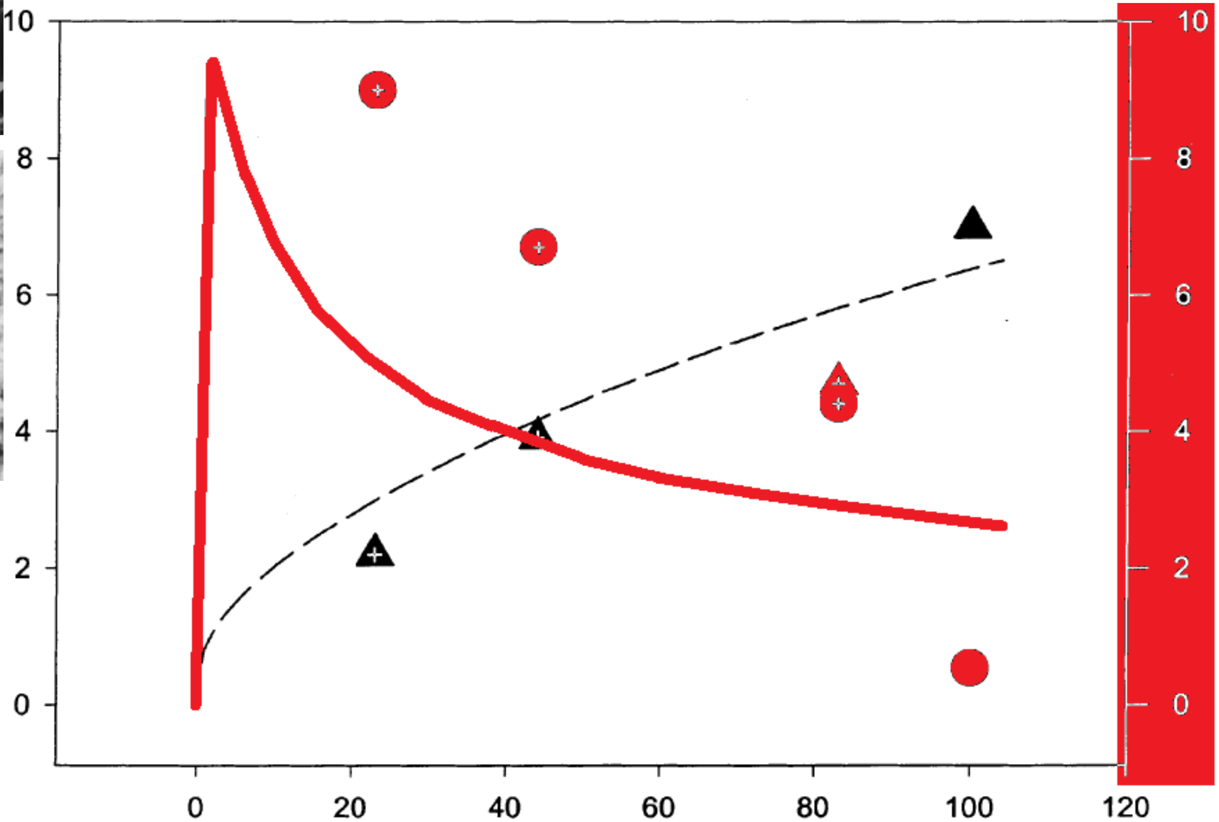
$$\frac{dc_v}{dt} = G - k_v^2 D_i c_i - k_i^2 D_v c_v - k_{vs}^2 D_v c_v$$

…….





Диаметр пузырей, нм



Плотность пузырей, 10^{23} м$^{-3}$

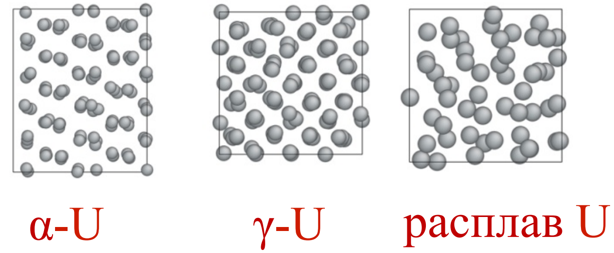
Выгорание, М*Вт*д/кг

Оксид. топливо: J. Nucl. Mat. 277, 231 (2000) & Металлич. топливо: J. Nucl. Mat. 425, 41 (2012)

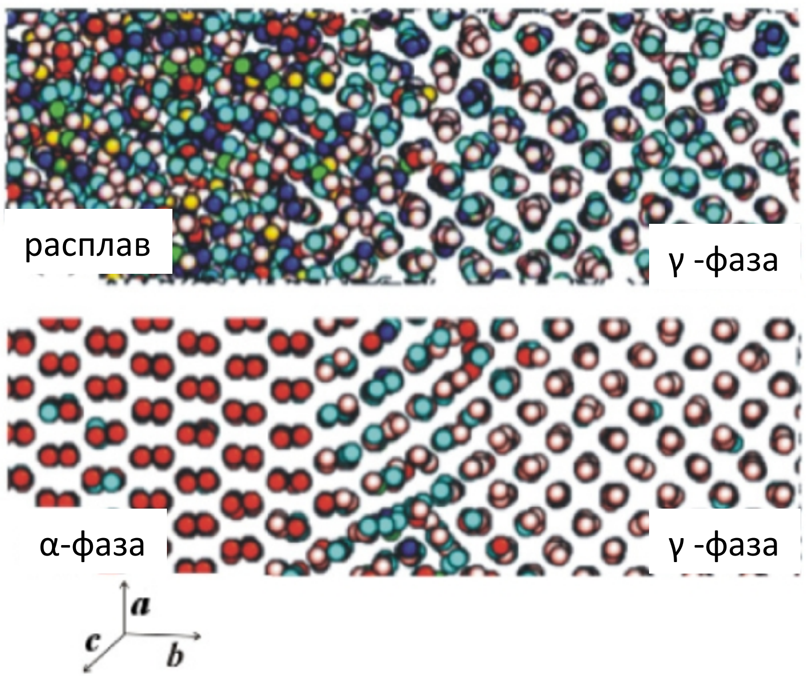
Многочастичный межатомный потенциал погруженного атома для системы U-Mo-Xe

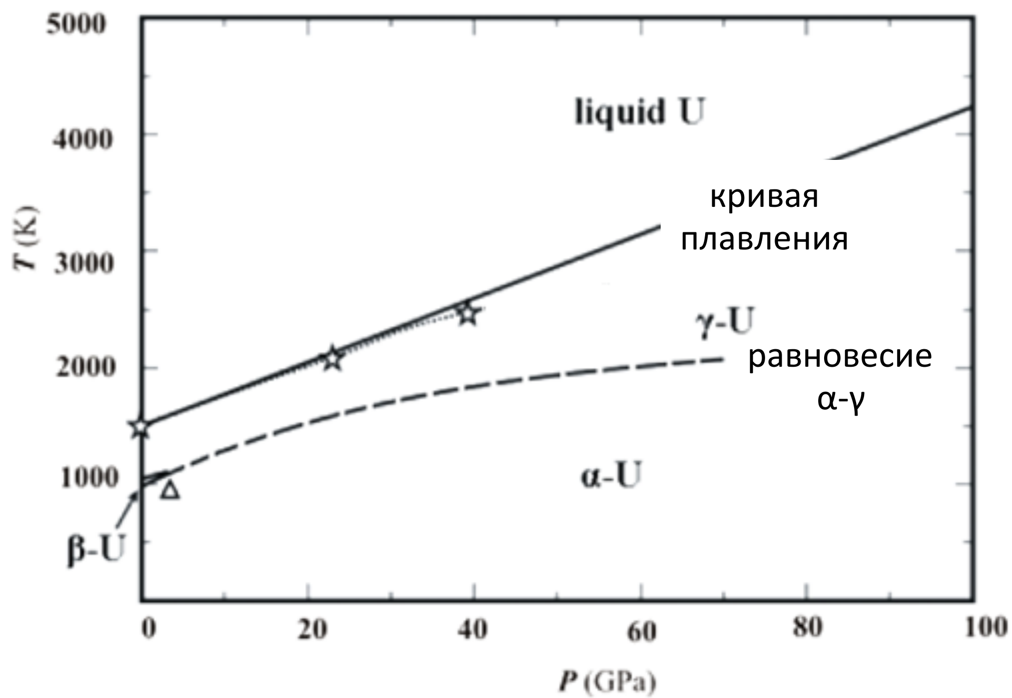
Потенциал создан впервые.

Полностью на основе ab-initio расчетов



Исследование фазовой диаграммы методом двухфазного равновесия





Хорошая точность описания фазовой диаграммы урана в широком диапазоне температур и давлений

J. Phys.: Condens. Matter 24, 015702 (**2012**)

Mod. & Sim. Mat. Sci. & Eng. 21, 035011 (**2013**)

уже 22 независимых цитирований

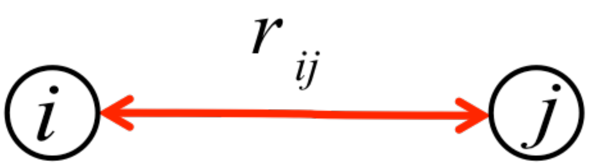
Органические жидкости (трансформаторные масла)

Н. Д. Кондратюк, В. В. Стегайлов, Г. Э. Норман. Микроскопические механизмы диффузии высших алканов // Высокомолекулярные соединения. Серия А. 2016. Т. 58, № 5, с. 519–531.

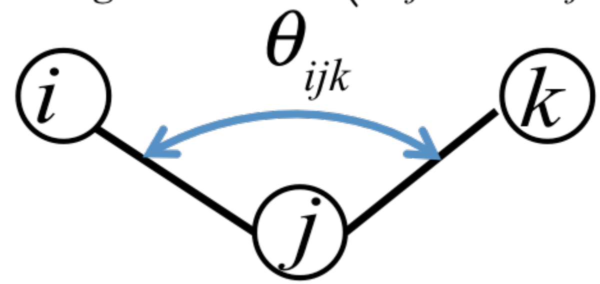
Межатомные и межмолекулярные взаимодействия

$$E = E_{bond} + E_{angle} + E_{dehedral} + E_{LJ} + E_{Coul}$$

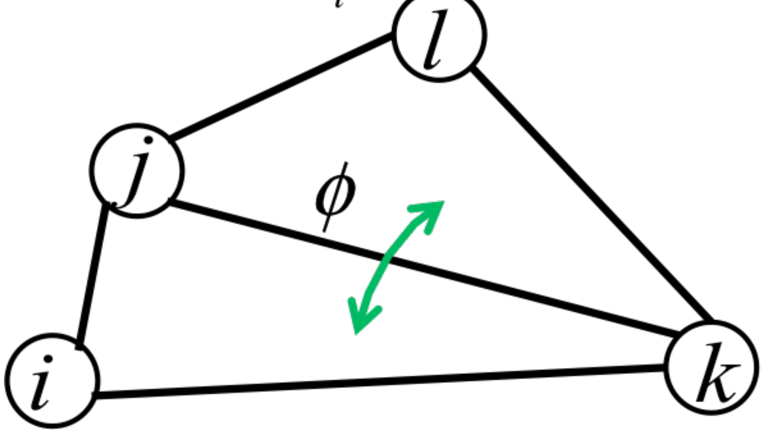
$$E_{bond} = K_b \left(r_{ij} - r_{ij}{}^{0}\right)^2$$



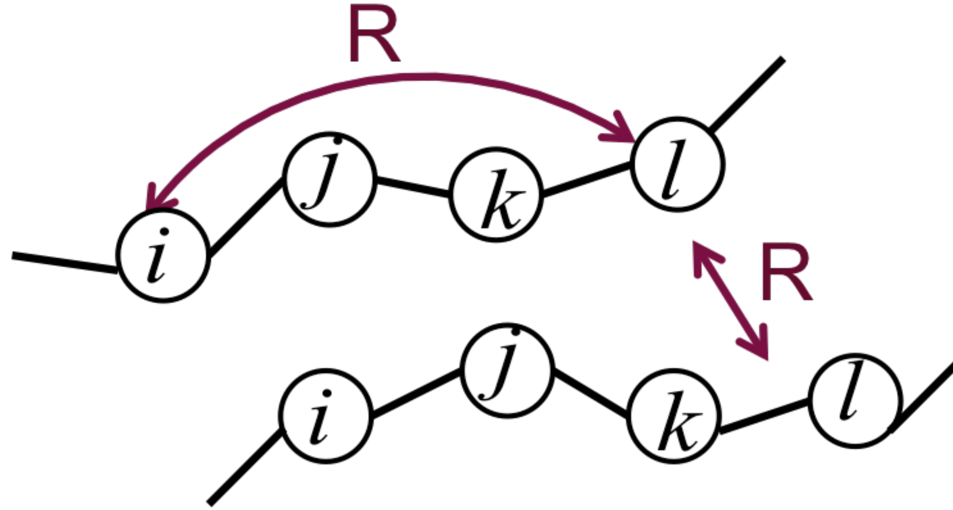
$$E_{angle} = K_a \left(\theta_{ijk} - \theta_{ijk}{}^{0}\right)^2$$



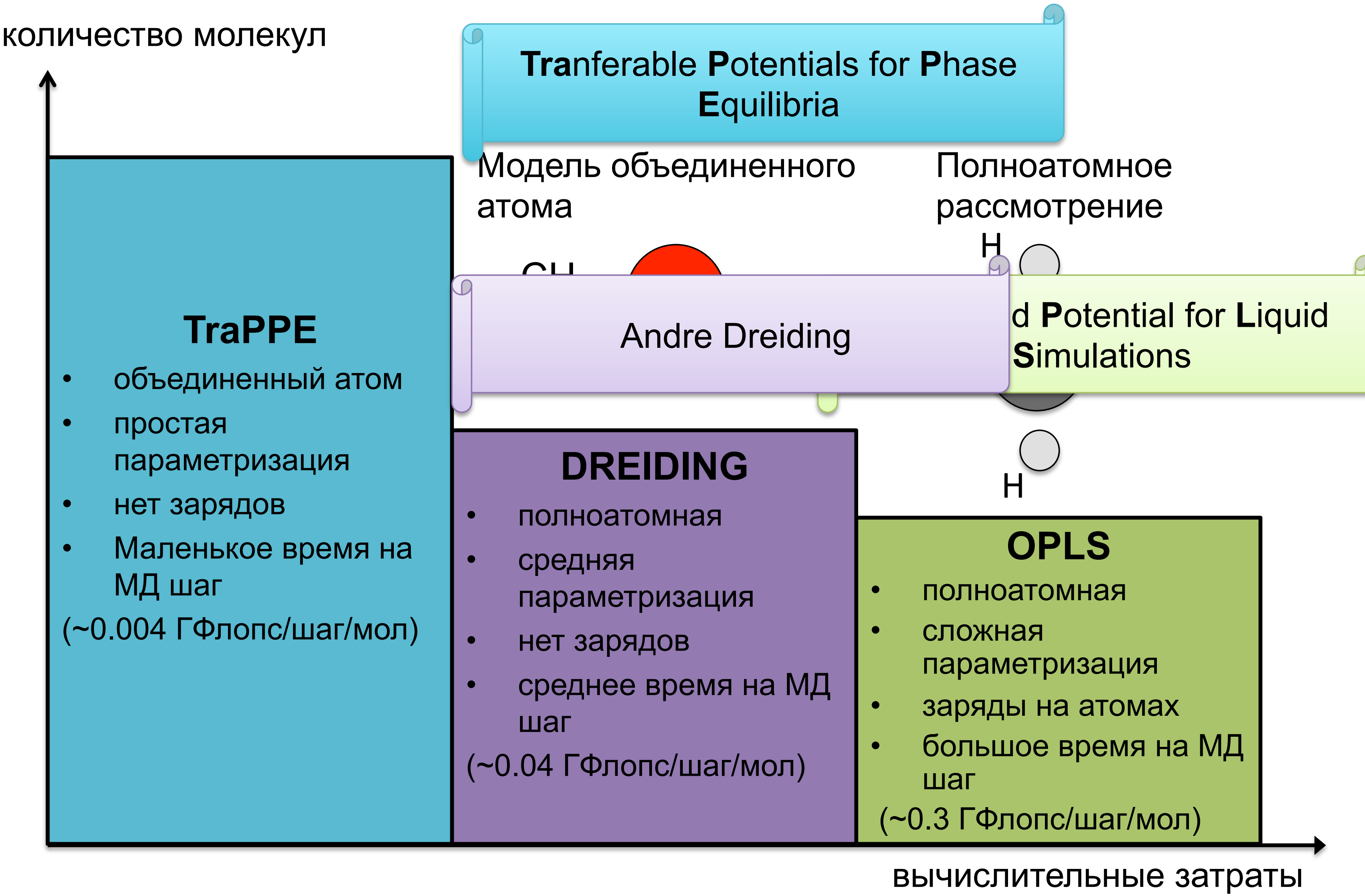
$$E_{dehedral} = \sum_i K_i [1 - \cos(i \cdot \phi)]$$



$$E_{LJ} = 4\varepsilon[(\sigma / R)^{12} - (\sigma / R)^{6}]$$



Различные приближения



Система

125-8000 молекул – TraPPE-UA (240000 атомов)

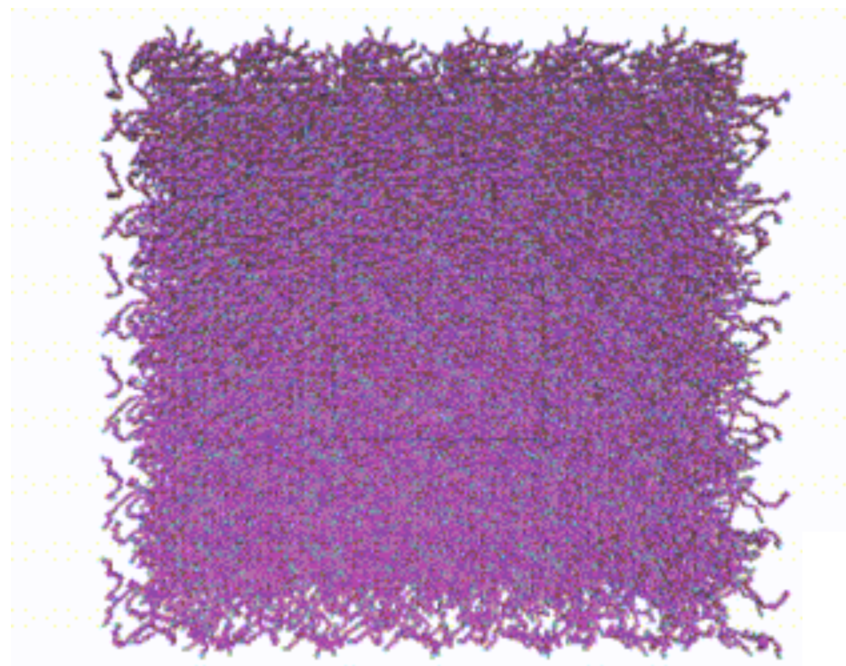
125-3375 молекул – DREIDING, OPLS (330000 атомов)

CH_3

CH_2

С. М.

$$\langle \Delta r^2 \rangle \qquad \langle v(0)v(t) \rangle$$



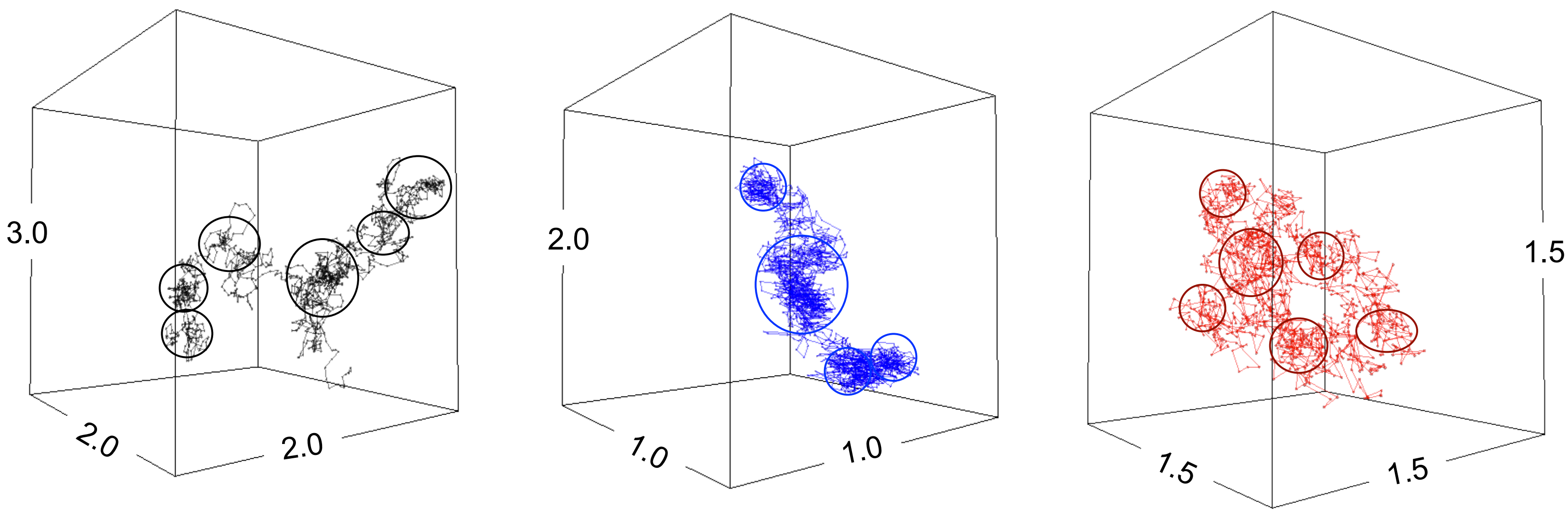
ρ = 0.77 g/cm^3

T = 353 K   P ~ 1 atm

L = 4.8 ÷ 19.2 nm

Аномальная диффузия

	TraPPE-UA	DREIDING	OPLS
Атомы H	✗	✔	✔
$E_{dehedral}$	$\sum K_i[1-\cos(i\cdot\phi)]$	$K[1+\cos(n\phi-d)]$	$\sum K_i[1-\cos(i\cdot\phi)]$
E_{Coul}	✗	✗	✔



D_{ES}, 10^{-6} см^2/с	5.40 ± 0.38	0.58 ± 0.04	1.90 ± 0.13

D_{exp} = 2.8 ± 0.14*

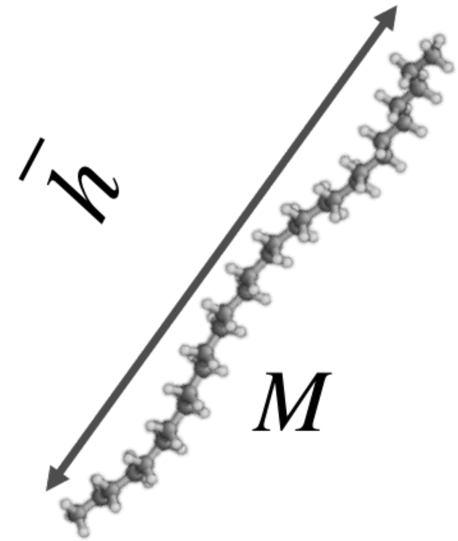
**Vardag, T., Karger, N., Lüdemann, H.D.* Temperature and Pressure Dependence of Self Diffusion in Long Liquid n-Alkanes. // *Berichte Der Bunsengesellschaft Für Physikalische Chemie*. 1991. V. 95. N. 8. P. 859.

Соотношение Стокса-Эйнштейна

$$\frac{D\eta}{k_B T} = \frac{1}{6\pi r}$$

Для полимеров*:

$$\frac{D\eta}{k_B T} = \frac{\rho}{36}\left(\frac{\overline{h}^2}{M}\right)$$



l(C-C) ~ 1.5 A

$M = 422.8$ g/mole

$\rho = 0.775$ g/cm^3

$T = 353$ K

$\overline{h} = 25$ A

	OPLS	Exp.
η, mPa*s	4.67	4.87**

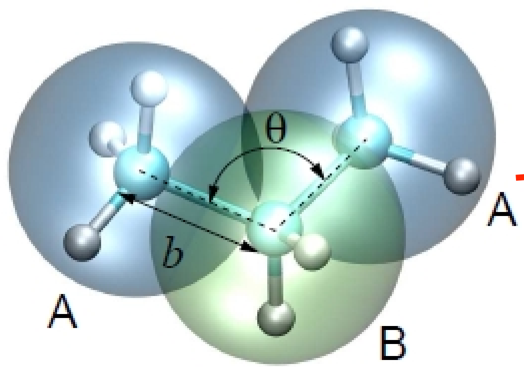
*Beuche F. *Viscosity, Self-Diffusion, and Allied Effects in Solid Polymers* // J. Chem. Phys. 1952.V. 20. N. 12. P. 1959

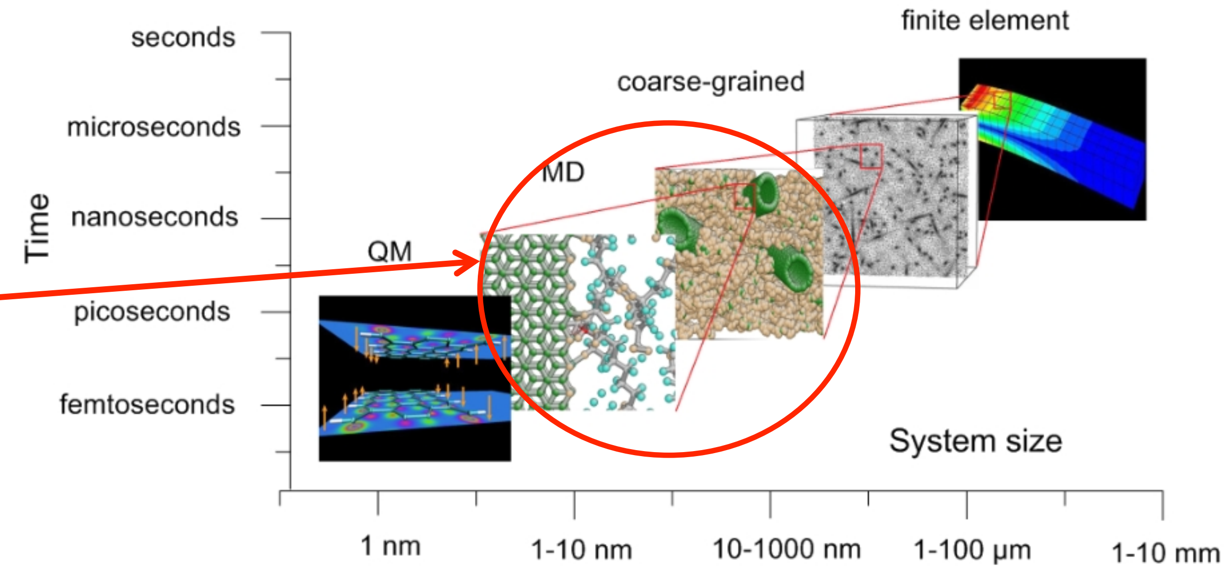
**Wohlfarth C. and Wohlfahrt B. 2002 Pure Organic Liquids vol 18B

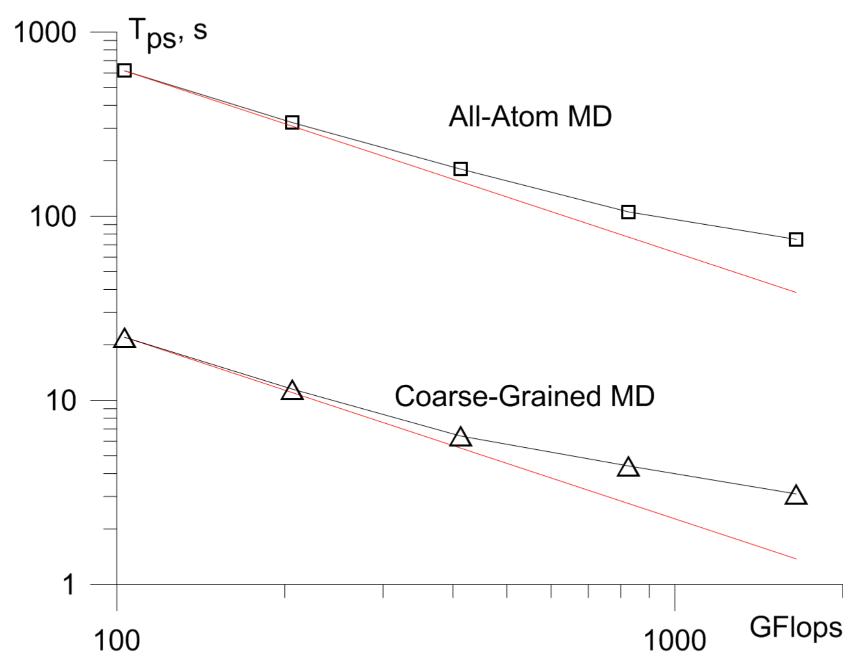
Полимерные композиты

Н. Д. Орехов, В. В. Стегайлов. Моделирование адгезионных свойств интерфейса полиэтилен - углеродная нанотрубка // Высокомолекулярные соединения. Серия А. 2016. Т. 58, № 3, с. 476–486.

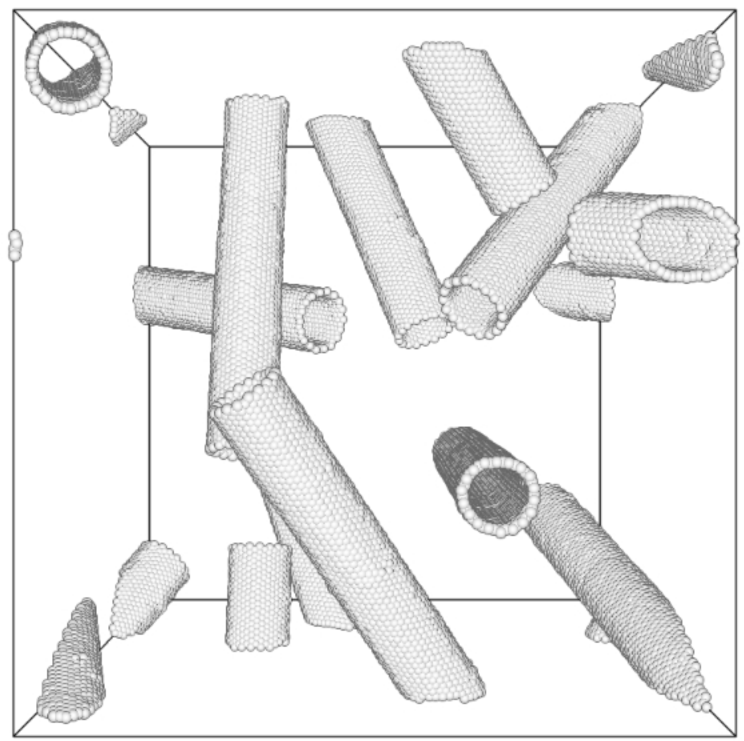
Coarse-grained Molecular Dynamics







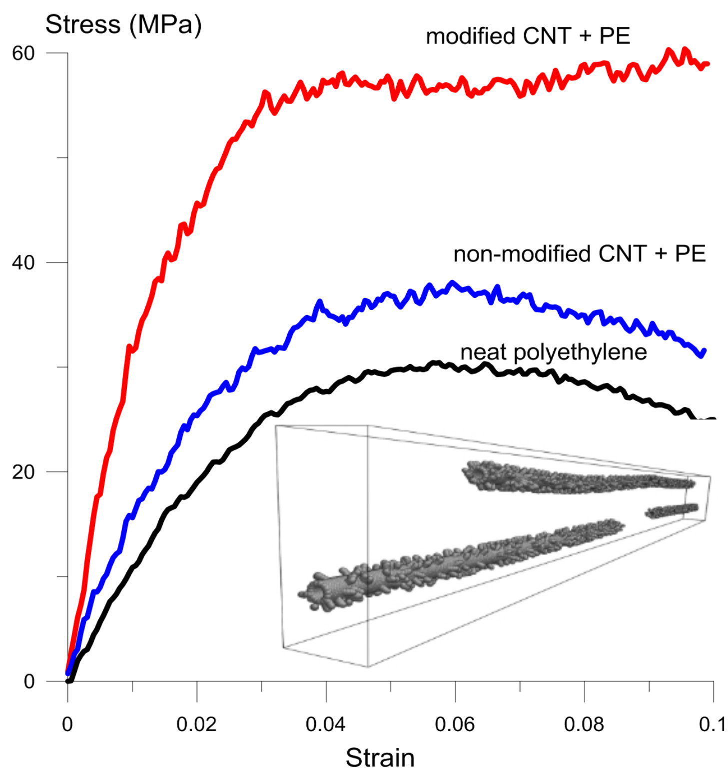
Nanocomposite deformation

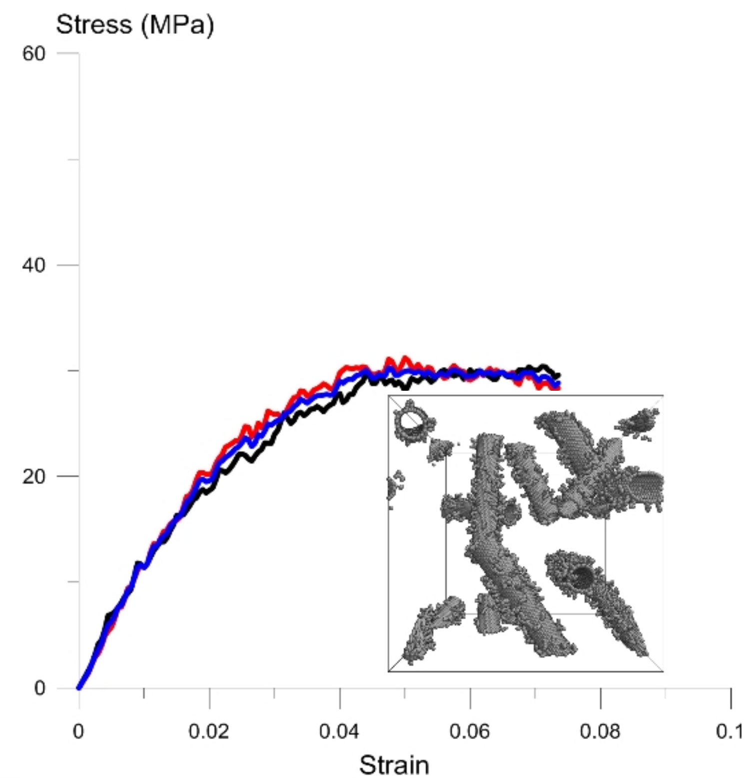


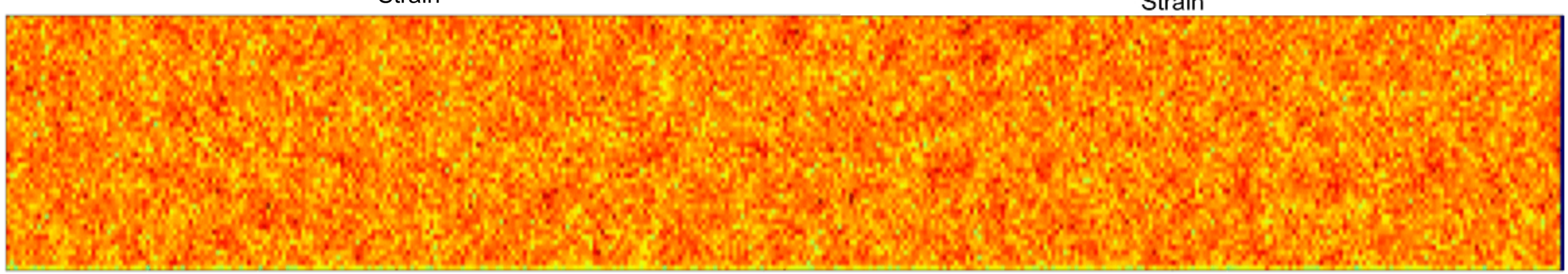
Nanocomposite deformation

Box size:	200x25x15 nm
CNT size:	175x2.5 nm
Aspect ratio:	70

Box size:	25x25x25 nm
CNT size:	20x2.5 nm
Aspect ratio:	8





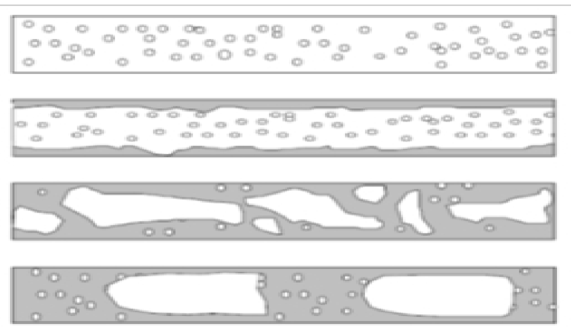


0.0 Strain

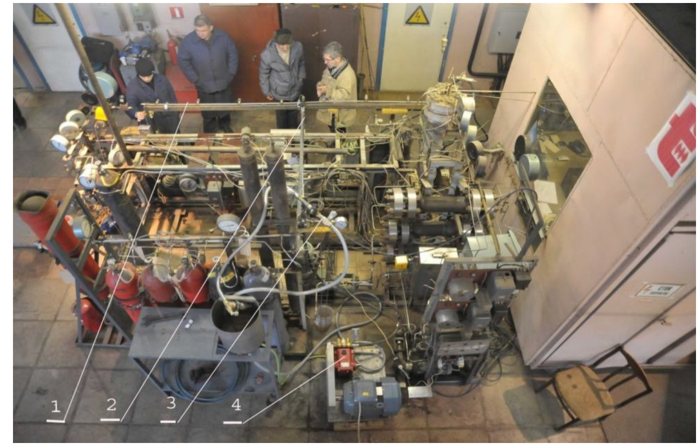
Газоконденсат
(фильтрация в пористых средах)

Norman, Genri E., Vasily V. Pisarev, Grigory S. Smirnov, and Vladimir V. Stegailov. "Atomistic Modeling and Simulation for Solving Gas Extraction Problems." In Foundations of Molecular Modeling and Simulation, pp. 137-151. Springer Singapore, 2016.

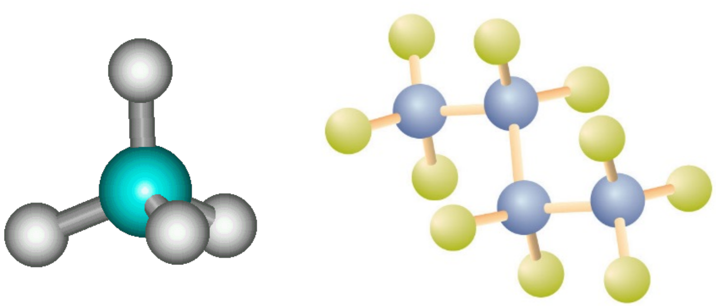
Мотивация работы



К гидродинамике двухфазных течений



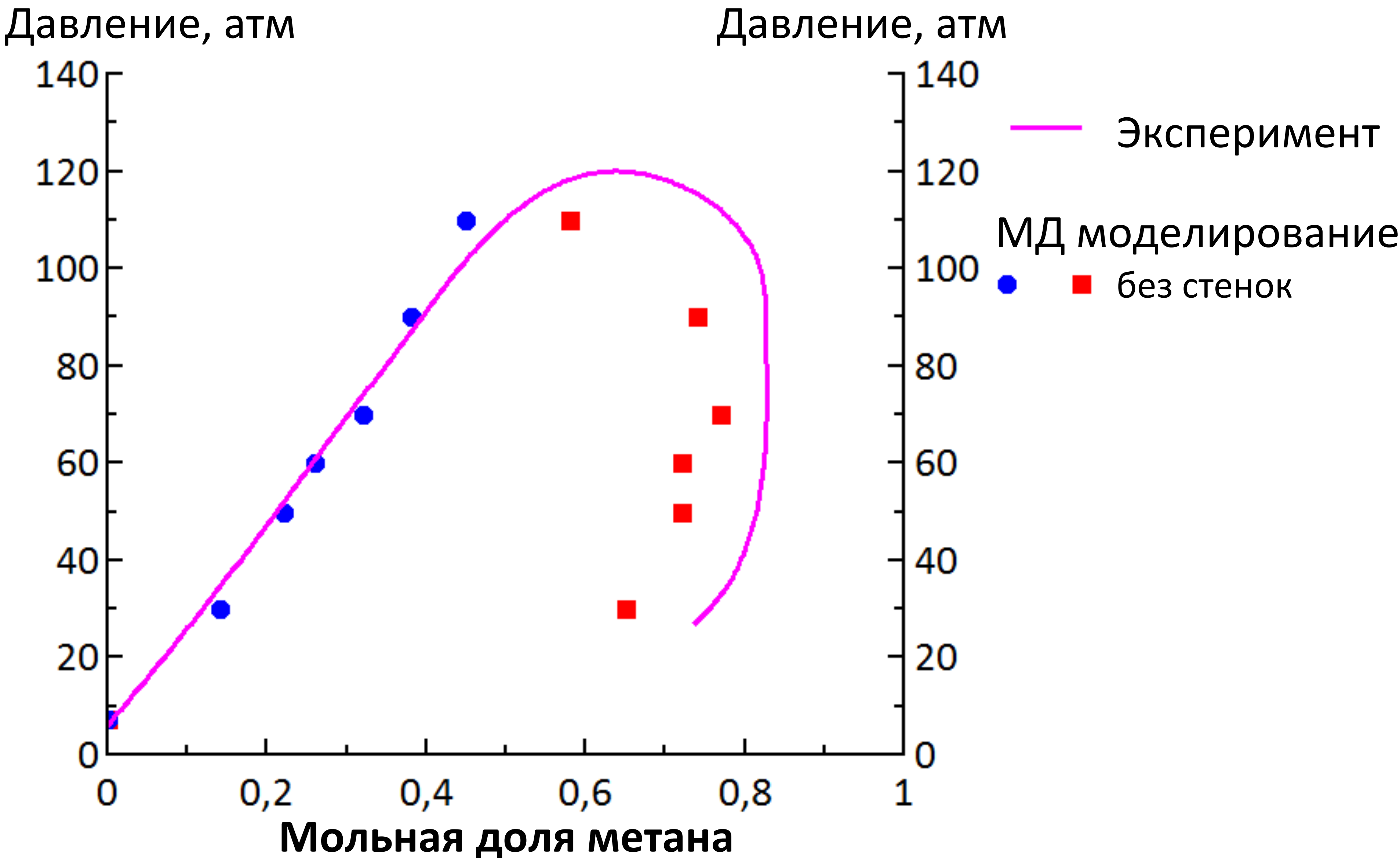
С экспериментальной проверкой (стенд «Пласт», ОИВТ РАН)



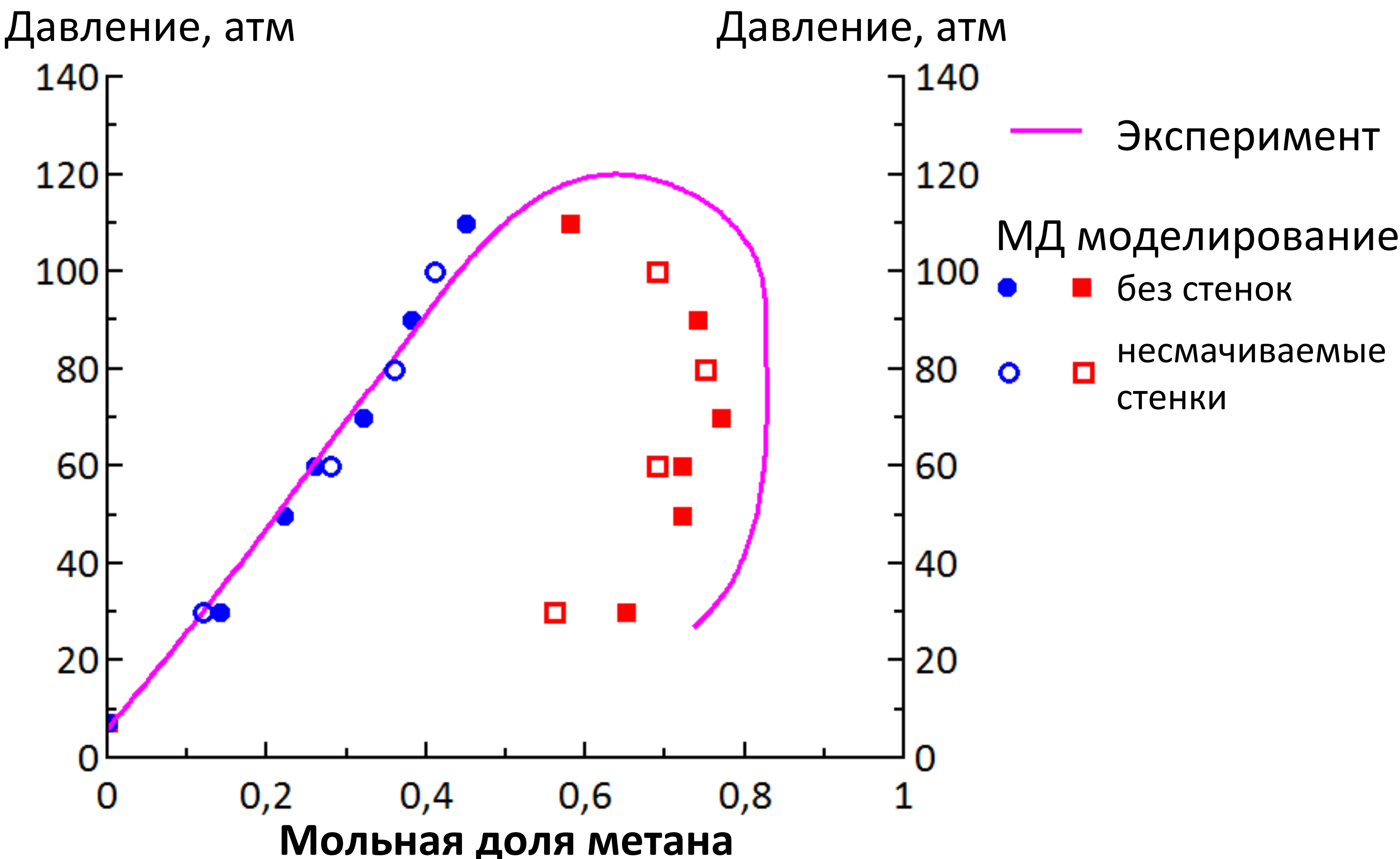
От атомистического моделирования

К решению одной из проблем газодобычи

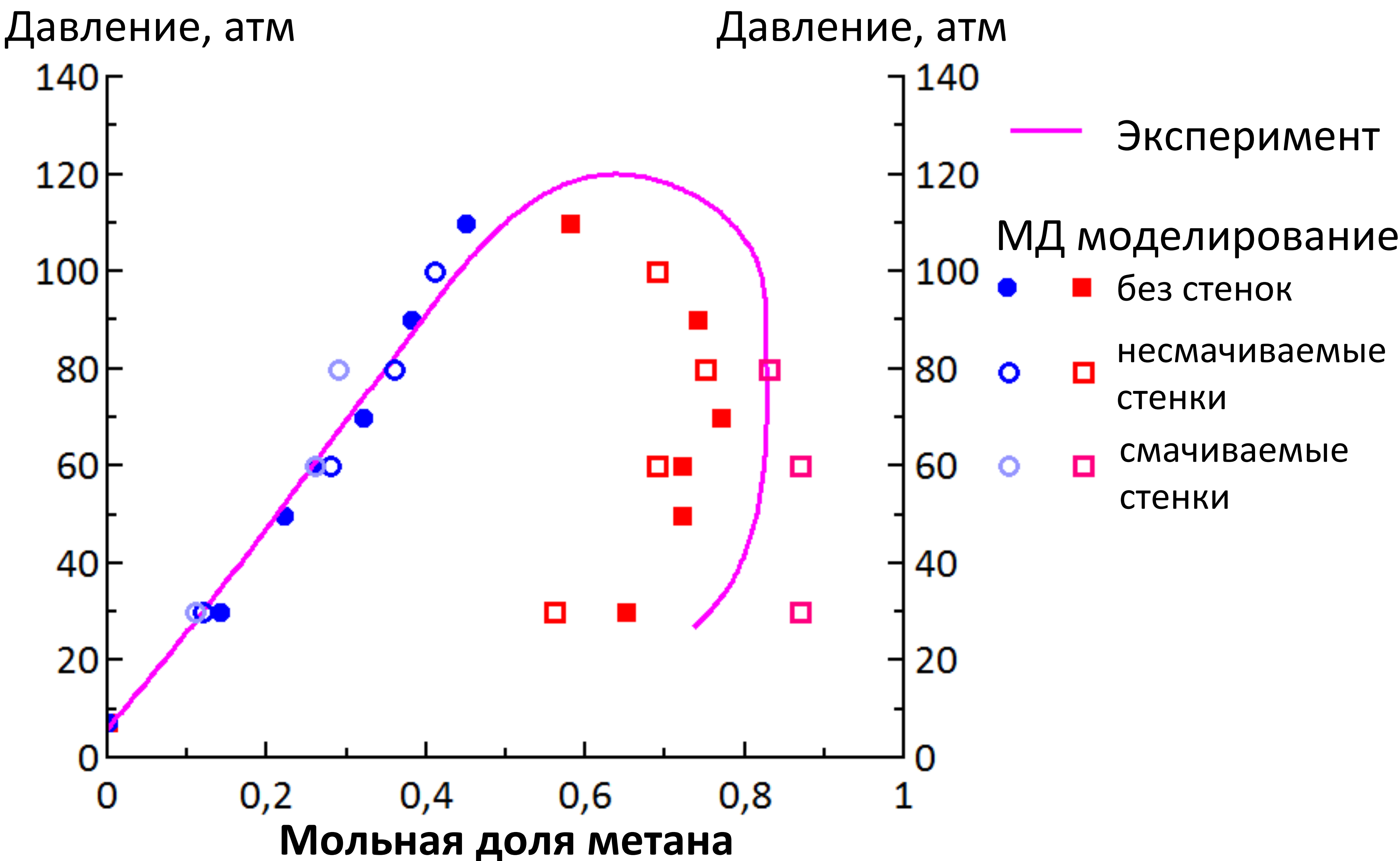
Сверхкритическая фазовая диаграмма (метан+бутан, 330 К, TraPPE-UA)



Сверхкритическая фазовая диаграмма (метан+бутан, 330 К, TraPPE-UA)



Сверхкритическая фазовая диаграмма (метан+бутан, 330 K, TraPPE-UA)



Газовые гидраты

фазовые диаграммы
кинетика образования и разложения

Smirnov G.S., Stegailov V.V. Melting and superheating of sI methane hydrate: Molecular dynamics study // Journal of Chemical Physics. 2012. V. 136. N. 4. P. 044523.

Smirnov G.S., Stegailov V.V. Toward Determination of the New Hydrogen Hydrate Clathrate Structures // Journal of Physical Chemistry Letters. 2013. V. 4. P. 3560-3564.

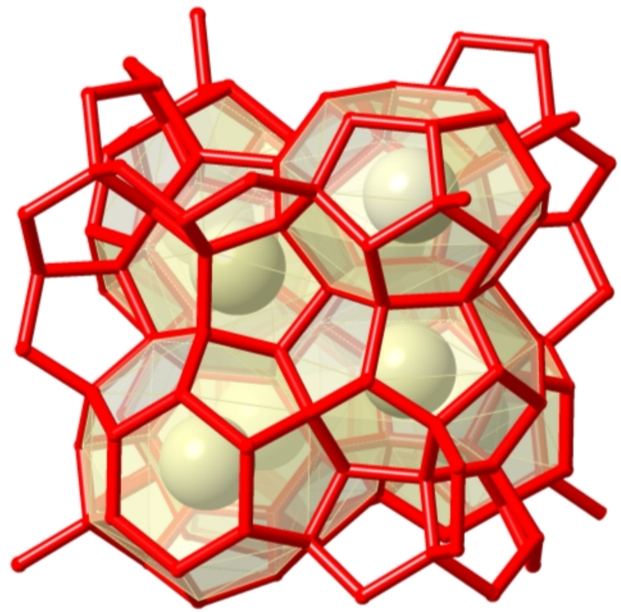
Methane Hydrates - Energy Source of the Future?

Estimated resource 1-5 million cubic kilometers of gas (500-2500 gigatones of carbon)

Lattice parameters of structure I

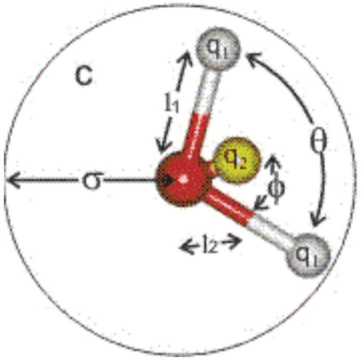
- Type: bcc
- Size ≈12x12x12 Å
- 8 methane molecules (100% cage occupancy)
- Elementary unit cell formula

$$(5^{12})_2 \cdot (5^{12}6^2)_6 \cdot 46\ H_2O$$

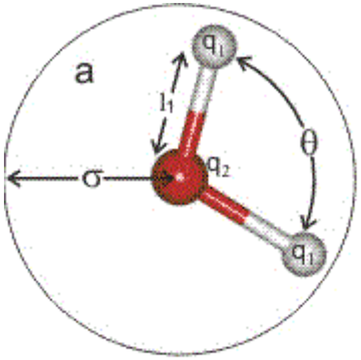


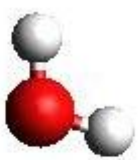
Interaction potentials for water

TIP4P - models



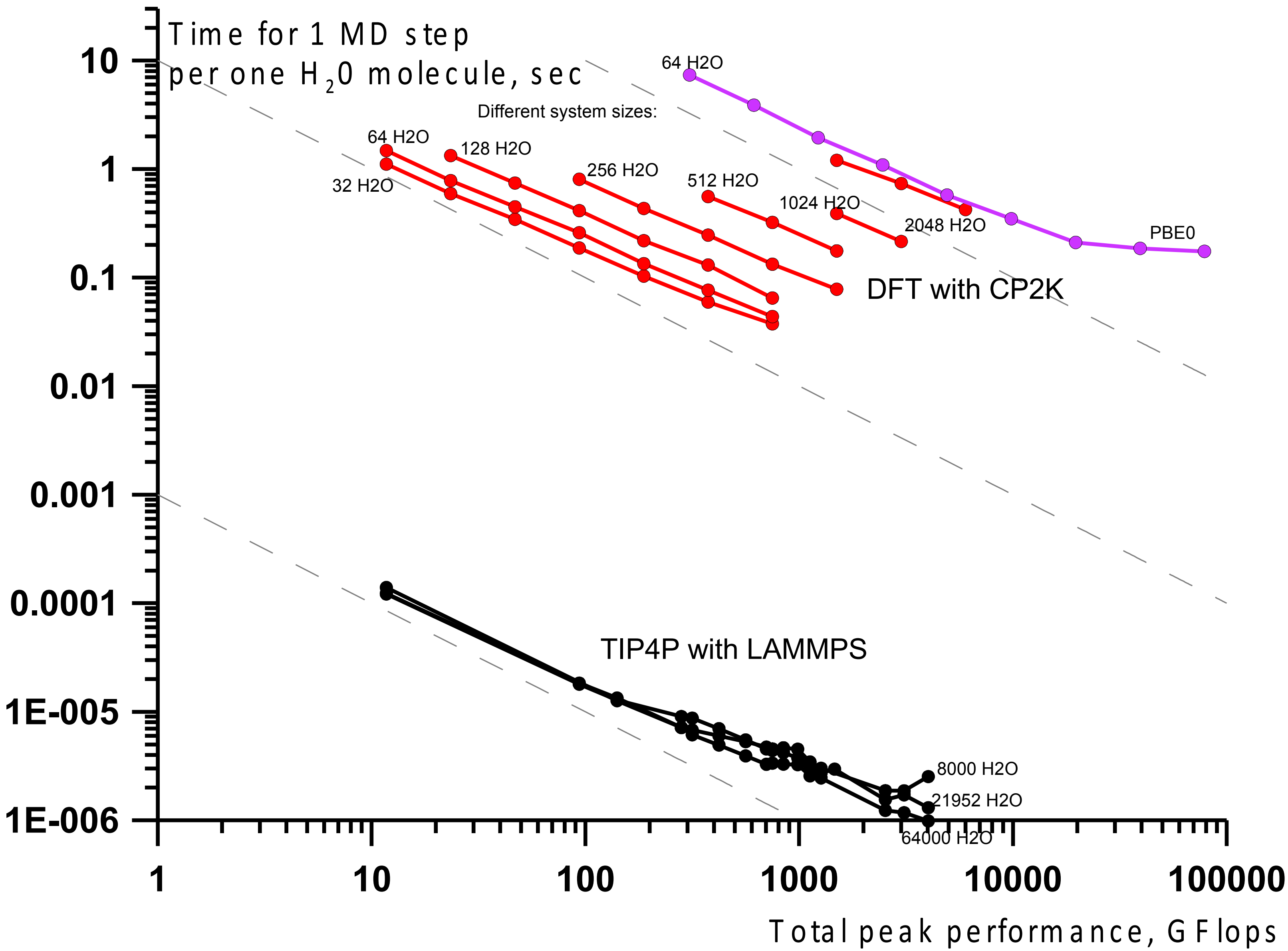
SPC/E





$$U_{ij} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right] + \frac{q_i q_j}{r}$$

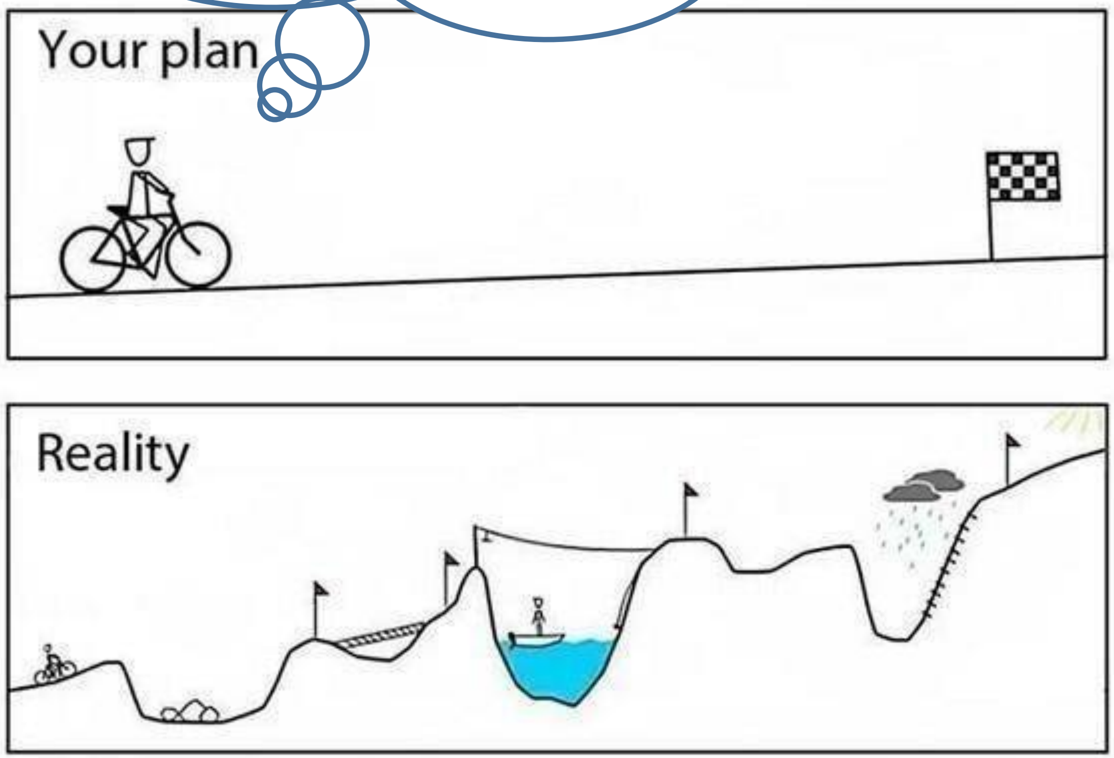
H_2O benchmark test with CP2K: comparison of different architectures

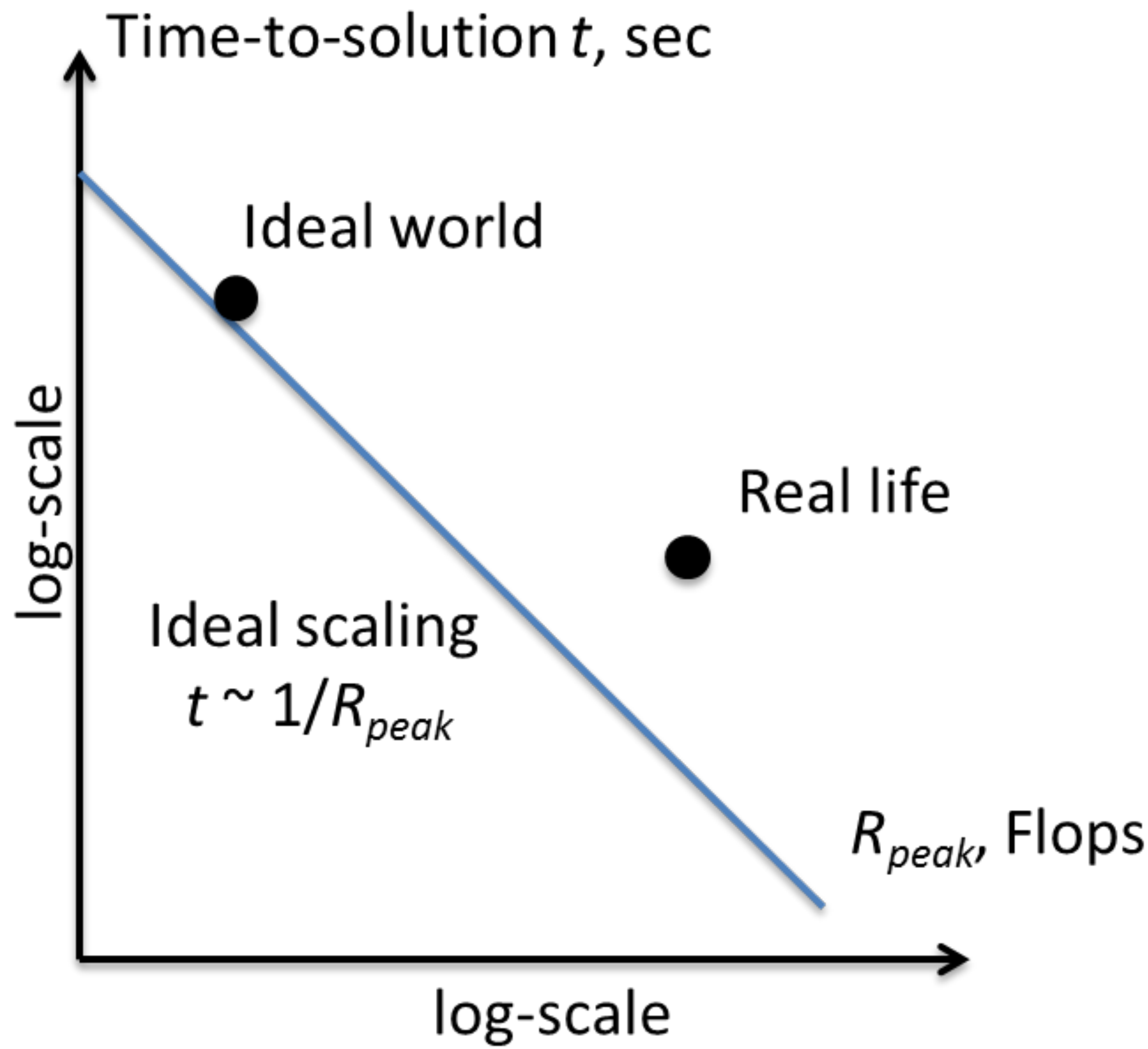


Путь к экзафлопсу

масштабируемость алгоритмов
и их адаптация к новому аппаратному обеспечению

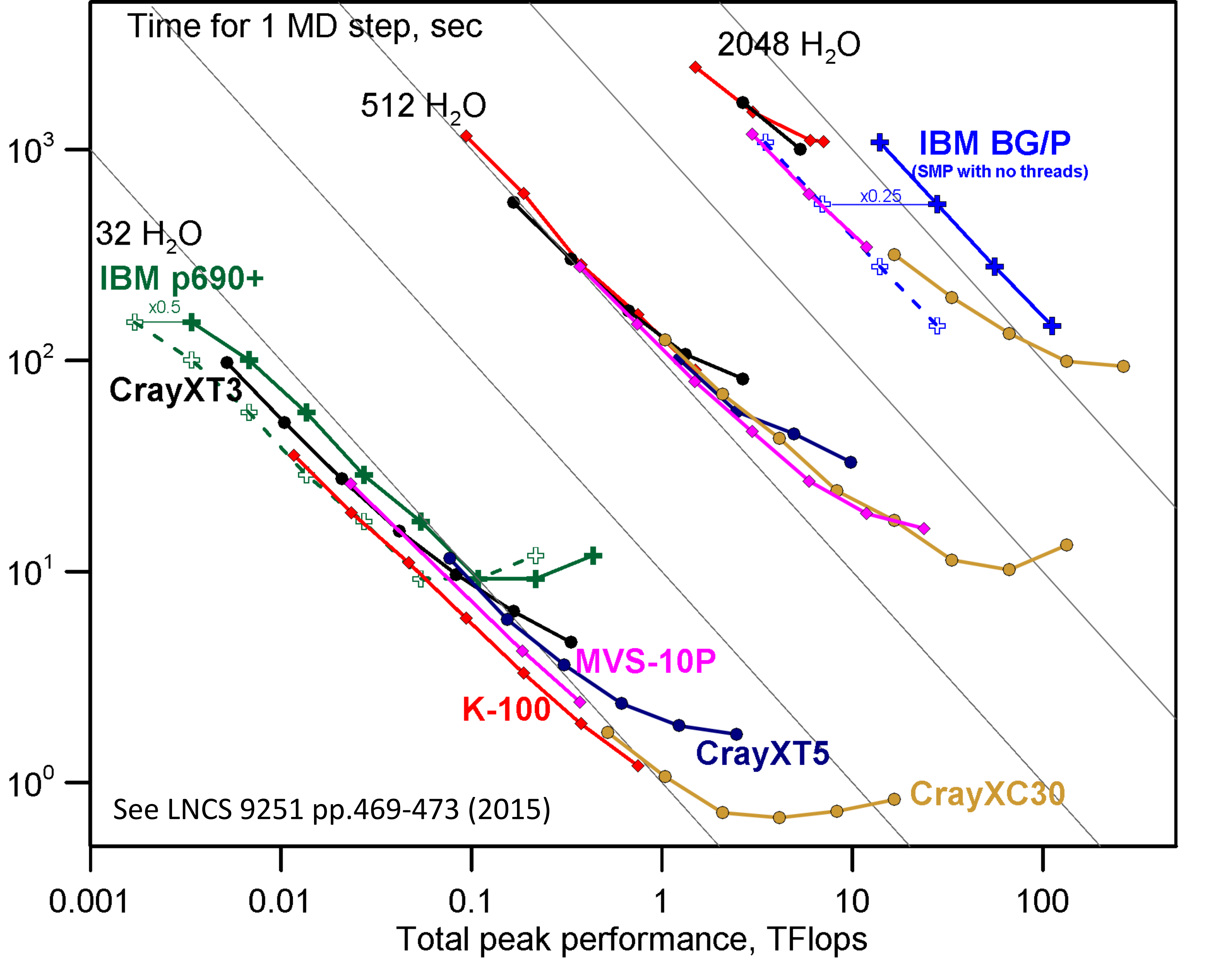
$$\text{Time-to-solution} \sim \frac{1}{R_{peak}}$$





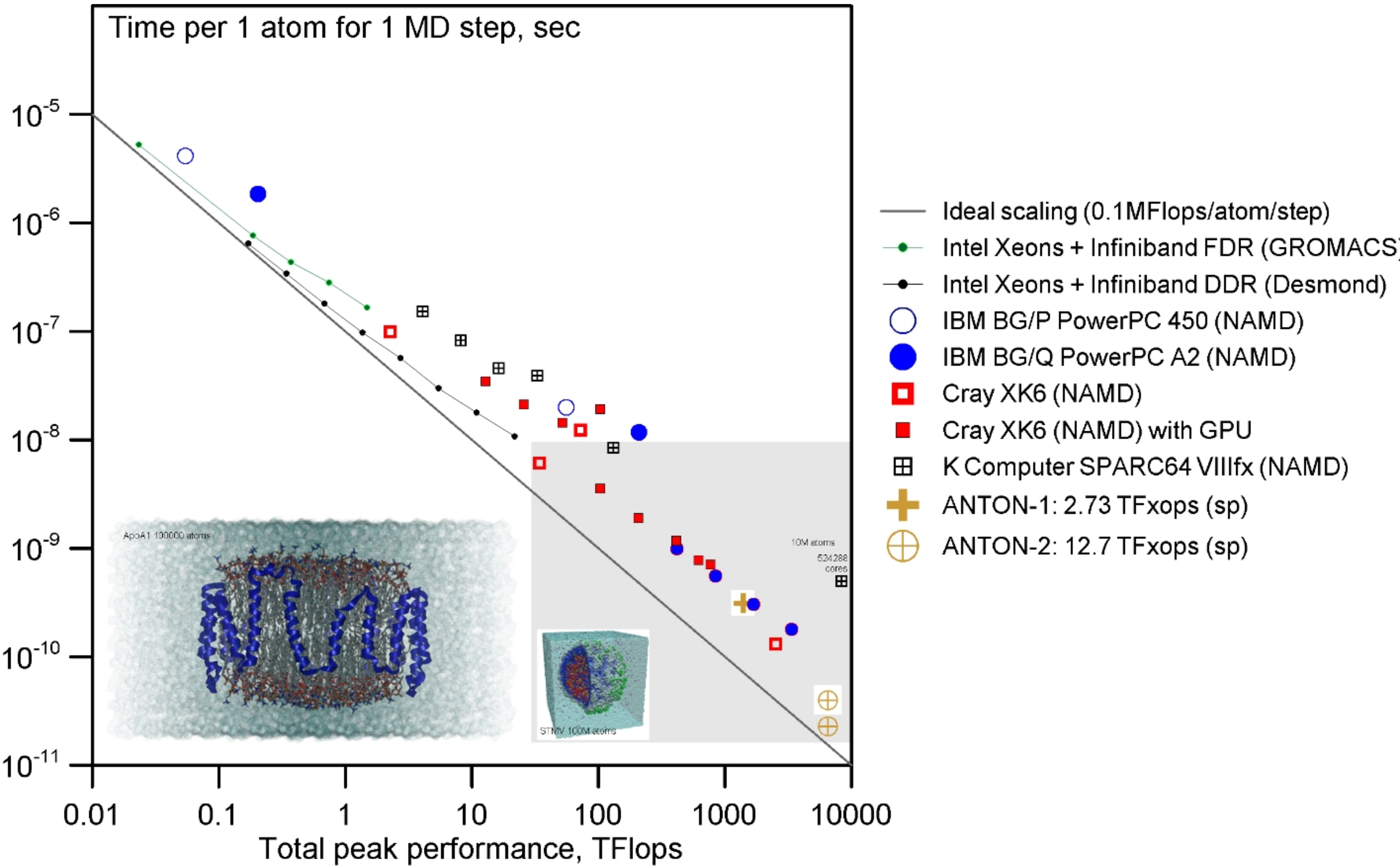
Vladimir V. Stegailov, Nikita D. Orekhov, and Grigory S. Smirnov,
HPC Hardware Efficiency for Quantum and Classical Molecular Dynamics
// V. Malyshkin (Ed.): PaCT 2015, LNCS 9251, pp. 469–473, 2015.

Ab initio
молекулярная динамика


Time for 1 MD step, sec
2048 H_2O
512 H_2O
32 H_2O
IBM BG/P
(SMP with no threads)
x0.25
IBM p690+
x0.5
CrayXT3
MVS-10P
K-100
CrayXT5
CrayXC30
See LNCS 9251 pp.469-473 (2015)
10^3
10^2
10^1
10^0
0.001
0.01
0.1
1
10
100
Total peak performance, TFlops

Классическая молекулярная динамика

Г. С. Смирнов, В. В. Стегайлов, “Эффективность алгоритмов классической молекулярной динамики на суперкомпьютерном аппаратном обеспечении”, Математическое моделирование, 28:5 (2016), 95–108



Time per 1 atom for 1 MD step, sec
10^-5
10^-6
10^-7
10^-8
10^-9
10^-10
10^-11
0.01
0.1
1
10
100
1000
10000
Total peak performance, TFlops
ApoA1 100000 atoms
STMV 100M atoms
10M atoms
524288 cores
Ideal scaling (0.1MFlops/atom/step)
Intel Xeons + Infiniband FDR (GROMACS)
Intel Xeons + Infiniband DDR (Desmond)
IBM BG/P PowerPC 450 (NAMD)
IBM BG/Q PowerPC A2 (NAMD)
Cray XK6 (NAMD)
Cray XK6 (NAMD) with GPU
K Computer SPARC64 VIIIfx (NAMD)
ANTON-1: 2.73 TFxops (sp)
ANTON-2: 12.7 TFxops (sp)

Доля гибридных систем: практичный взгляд

CORAL Joint NNSA & SC Leadership Computing Acquisition Project

Current DOE Leadership Computers

Titan (ORNL)
2012 - 2017

Sequoia (LLNL)
2012 - 2017

Mira (ANL)
2012 - 2017

Objective - Procure 3 leadership computers to be sited at ANL, ORNL, and LLNL in CY17-18

Leadership Computers run the most demanding DOE mission applications and advance HPC technologies to assure continued US/DOE leadership

Approach:

Competitive process - one RFP (issued by LLNL) leading to 2 Non-Recurring Engineering (NRE) contracts and 3 computer procurement contracts

For risk reduction and to meet a broad set of requirements,
2 architectural paths will be selected – one at each of the LCF centers.

Once selected, multi-year, lab-awardee relationship to deliver the best performance

Both NRE contracts jointly managed by the 3 Labs

Each lab manages and negotiates its own computer procurement contract, and may exercise options to meet their specific needs

Understanding that **long procurement lead time may impact architectural characteristics and designs** of procured computers

Susan Coghlan, **ALCF** & Arthur Bland, **OLCF**, presented to **ASCAC** of DOE

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
9	Forschungszentrum Juelich (FZJ) Germany	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458,752	5,008.9	5,872.0	2,301
20	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR IBM/Lenovo	147,456	2,897.0	3,185.1	3,422.7
21	Leibniz Rechenzentrum Germany	**SuperMUC Phase 2** - IBM NeXtScale nx360M5, Xeon E5-2697v3 14C 2.6GHz, Infiniband FDR14 Lenovo/IBM	86,016	2,813.6	3,578.3	1,480.8
23	HLRS - Höchstleistungsrechenzentrum Stuttgart Germany	**Hornet** - Cray XC40, Xeon E5-2680v3 12C 2.5GHz, Aries interconnect Cray Inc.	94,608	2,763.0	3,784.3	1,512
47	Max-Planck-Gesellschaft MPI/IPP Germany	iDataPlex DX360M4, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband FDR IBM	65,320	1,283.3	1,463.2	1,260
56	DKRZ - Deutsches Klimarechenzentrum Germany	**Mistral** - bullx DLC 720, Xeon E5-2680v3 12C 2.5GHz, Infiniband FDR Bull, Atos Group	37,344	1,139.2	1,493.8	
66	TU Dresden, ZIH Germany	**Taurus** - bullx DLC 720, Xeon E5-2680v3 12C 2.5GHz, Infiniband FDR Bull, Atos Group	34,656	1,029.9	1,386.2	620
69	HLRN at ZIB/Konrad Zuse-Zentrum Berlin Germany	**Konrad** - Cray XC40, Intel Xeon E5-2695v2/E5-2680v3 12C 2.4/2.5GHz, Aries interconnect Cray Inc.	44,928	991.5	1,425.7	
82	HWW/Universitaet Stuttgart Germany	**HERMIT** - Cray XE6, Opteron 6276 16C 2.30 GHz, Cray Gemini interconnect Cray Inc.	113,472	831.4	1,043.9	
83	HLRN at Universitaet Hannover / RRZN Germany	**Gottfried** - Cray XC40, Intel Xeon E5-2695v2 12C 2.4GHz/E5-2680v3 12C 2.5GHz, Aries interconnect Cray Inc.	40,320	829.8	1,241.4	
102	Max-Planck-Gesellschaft MPI/IPP Germany	iDataPlex DX360M4, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband, NVIDIA K20x IBM	15,840	709.7	1,013.1	269.9

Текущая доля гибридных систем

Реальная эффективность гибридных систем по сравнению с обычными суперкомпьютерами, основанными на обычных ЦПУ может быть проиллюстрирована списком самых крупных суперкомпьютеров Франции и Германии в текущем списке Топ500.

Франция:
14 систем (номера в Топ500 29, 36, 44, 60, 64, 98, 127, 130, 140, 142, 153, 184, 189, 278) основаны на обычных ЦПУ, главным образом Intel Xeon. Их **полная пиковая мощность Rpeak = 13.5 ПФлопс**.
И только 15-я система номер 279 имеет GPU ускорители. (**Rpeak = 0.38 ПФлопс**)

Германия:
10 систем (номера в Топ500 9, 20, 21, 23, 47, 56, 66, 69, 82, 83) основаны на обычных ЦПУ, главным образом Intel Xeon. Их **полная пиковая мощность Rpeak = 24 ПФлопс**.
И только 11-я система номер 102 имеет GPU ускорители Nvidia. (**Rpeak = 1 ПФлопс**)

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,659.9
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
6	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115,984	6,271.0	7,788.9	2,325
7	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462,462	5,168.1	8,520.1	4,510
8	Forschungszentrum Juelich (FZJ) Germany	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458,752	5,008.9	5,872.0	2,301
9	DOE/NNSA/LLNL United States	**Vulcan** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	393,216	4,293.3	5,033.2	1,972
10	Government United States	Cray CS-Storm, Intel Xeon E5-2660v2 10C 2.2GHz, Infiniband FDR, Nvidia K40 Cray Inc.	72,800	3,577.0	6,131.8	1,498.9

Топ10 из Топ500
Ноябрь 2014

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,659.9
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
6	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115,984	6,271.0	7,788.9	2,325
7	King Abdullah University of Science and Technology Saudi Arabia	**Shaheen II** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	196,608	5,537.0	7,235.2	2,834
8	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462,462	5,168.1	8,520.1	4,510
9	Forschungszentrum Juelich (FZJ) Germany	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458,752	5,008.9	5,872.0	2,301
10	DOE/NNSA/LLNL United States	**Vulcan** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	393,216	4,293.3	5,033.2	1,972

Топ10 из Топ500
Июнь 2015

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,659.9
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
6	DOE/NNSA/LANL/SNL United States	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	301,056	8,100.9	11,078.9	
7	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115,984	6,271.0	7,788.9	2,325
8	HLRS - Höchstleistungsrechenzentrum Stuttgart Germany	**Hazel Hen** - Cray XC40, Xeon E5-2680v3 12C 2.5GHz, Aries interconnect Cray Inc.	185,088	5,640.2	7,403.5	
9	King Abdullah University of Science and Technology Saudi Arabia	**Shaheen II** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Aries interconnect Cray Inc.	196,608	5,537.0	7,235.2	2,834
10	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462,462	5,168.1	8,520.1	4,510

Топ10 из Топ500
Ноябрь 2015

Conclusions

- Atomistic and continuum models shares 1/3 and 1/3 in the distribution of computational time from the US DOE perspective.
- Quantum and classical atomistic models represent a wide spectrum of important problems that require petascale performance. There are examples of effective deployment of such systems.
- Quantum MD takes about >60% of computational time at some supercomputer centers.
  However the corresponding algorithms are being adapted to the hybrid architectures quite slowly.
  The interconnect is the key technology.
- The efficiency of the special methods of performance increase (FMA, SIMD) needs careful consideration for the particular problems/algorithms.
- Statistics shows that in the countries that do not produce hybrid hardware the current rationally estimated proportion of hybrid systems is not higher than 5%.